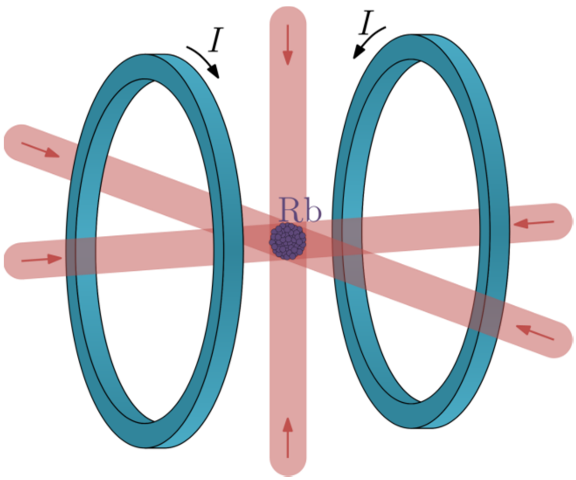
Molecular dynamics simulations for laser-cooled sources

Bas van der Geer
Marieke de Loos
Pulsar Physics

Edgar Vredenbregt
Wouter Engelen
Jom Luiten
and many others
Eindhoven University

The Netherlands

Ultracold Electron/Ion Source

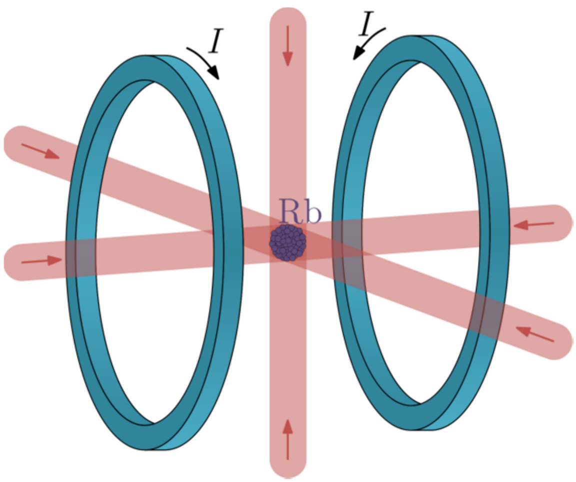


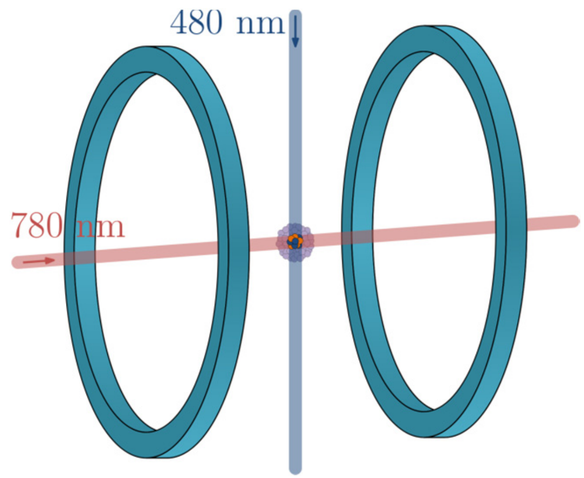
Trap & Cool

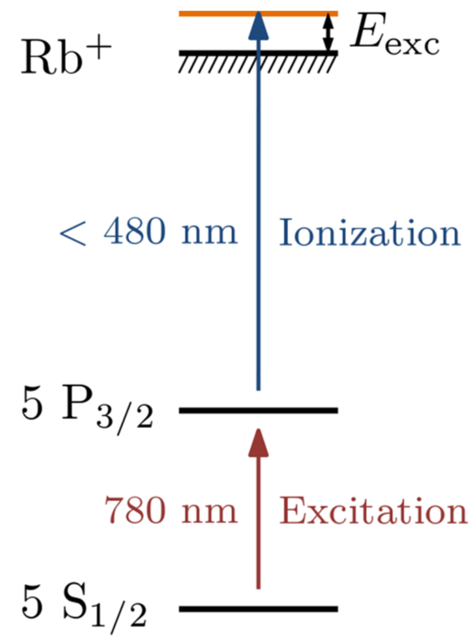
Magneto-optical trap

Density ≈ 10^{16} / m^3
RMS size ≈ 1 mm
T = 100 μK

Ultracold Electron/Ion Source







Trap & Cool

Magneto-optical trap

Density ≈ 10^{16} / m^3
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T = 100 ⌈K

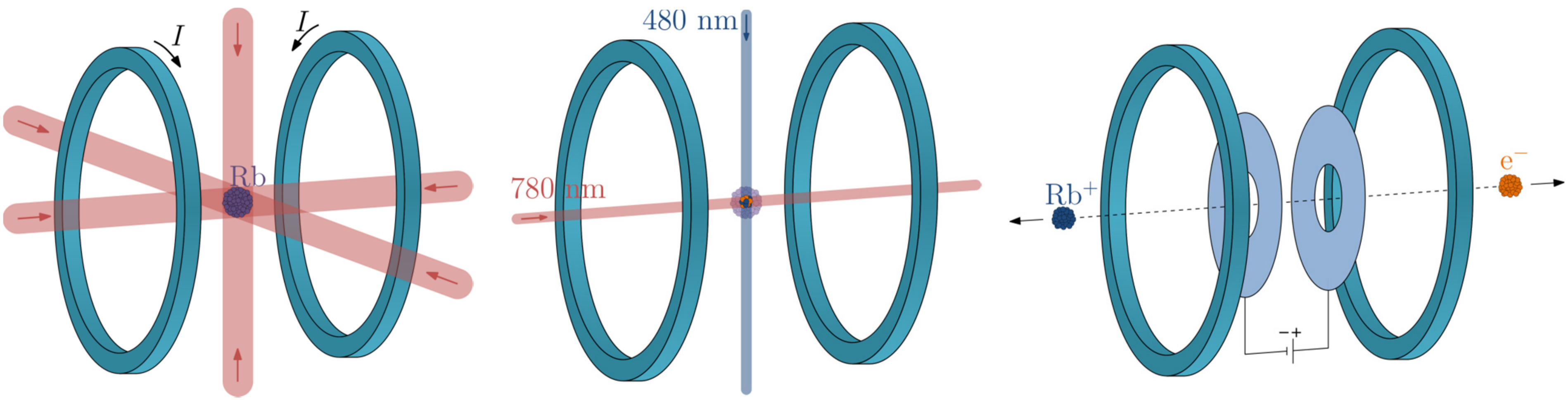
Ionize

Ultracold plasma

Ionization radius ≈ 50 µm

Killian et al.,
PRL 83, 4776 (1999)

Ultracold Electron/Ion Source



Trap & Cool

Magneto-optical trap

Density ≈ 10^{16} / m^3
RMS size ≈ 1 mm
T = 100 μK

Ionize

Ultracold plasma

Ionization radius ≈ 50 μm

Killian et al.,
PRL 83, 4776 (1999)

Accelerate

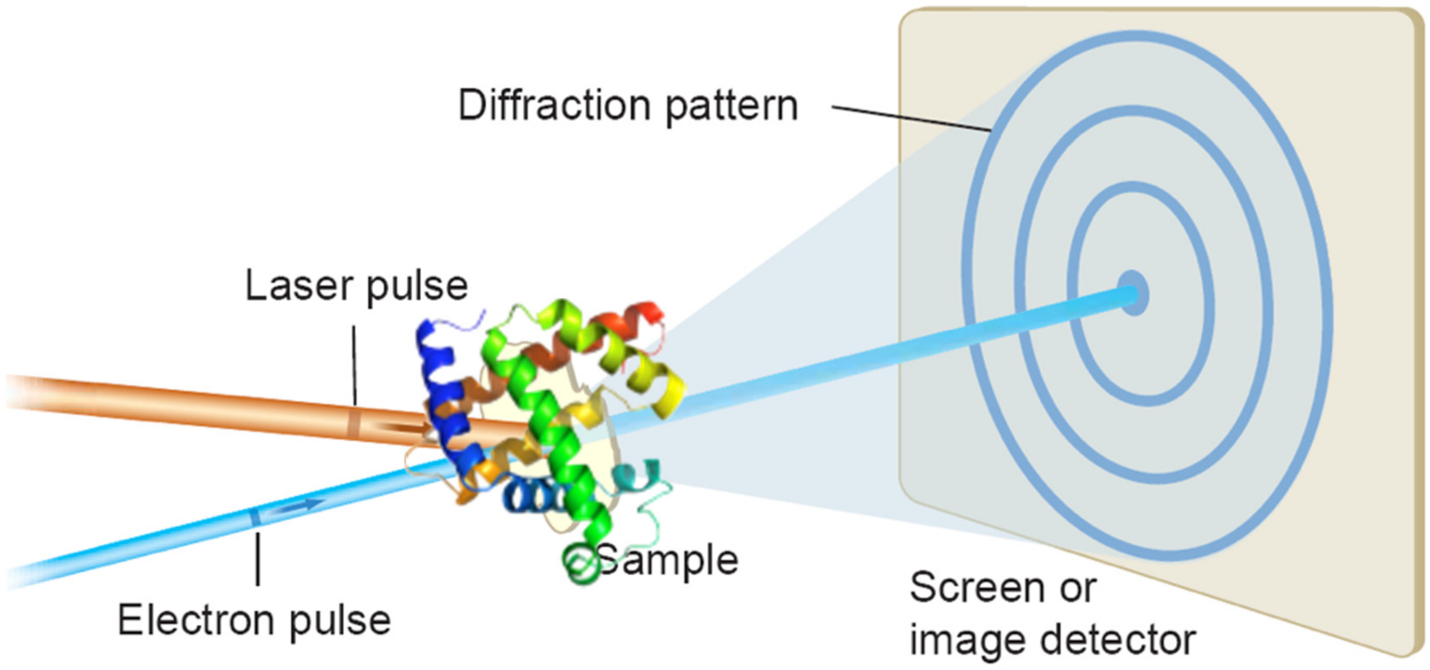
Ultracold source

Bunch energy E = 15 keV

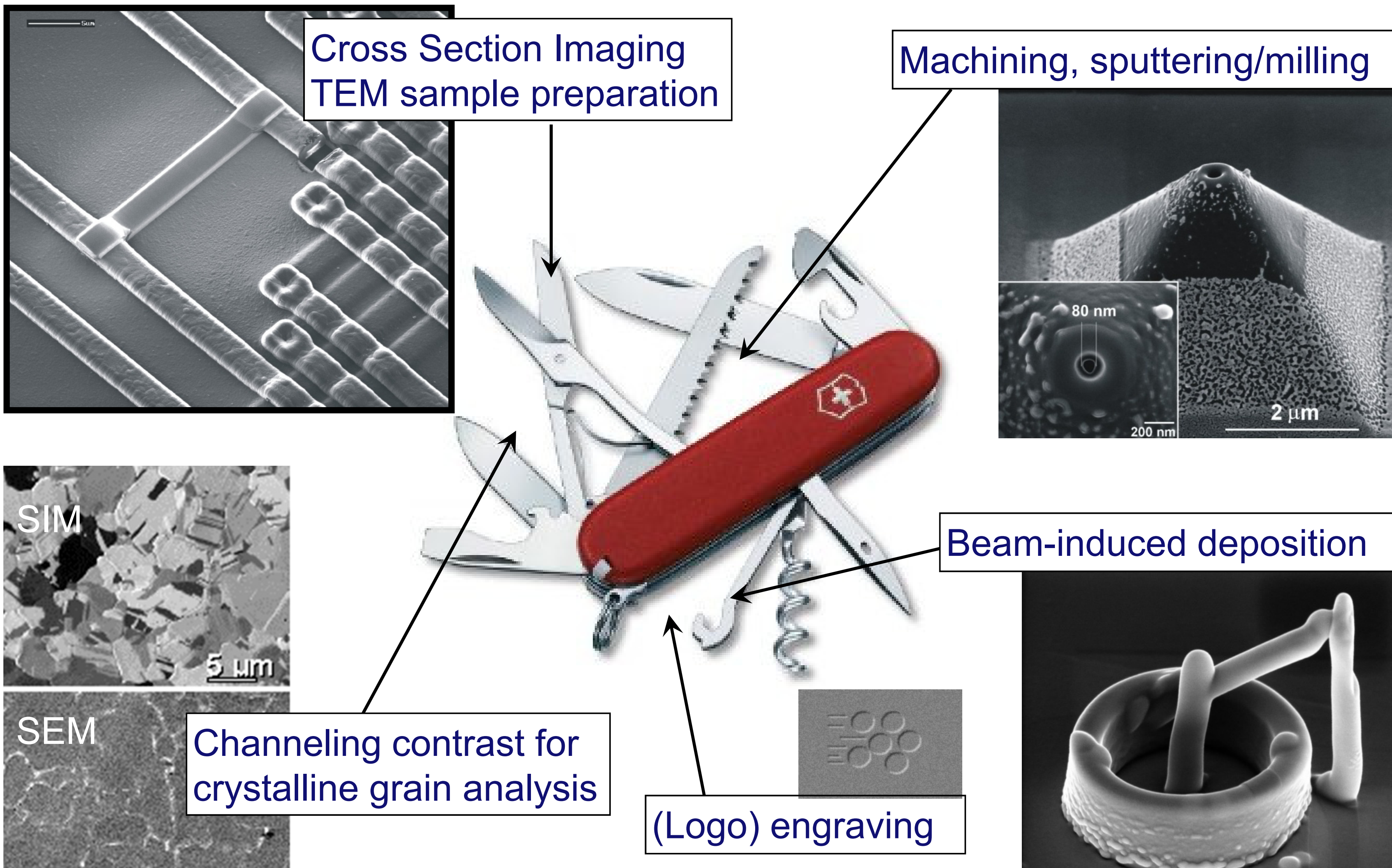
Luiten et al.,
PRL 95, 164801 (2005)
McCulloch et al.,
Nat. Phys. 7, 785 (2011)

Application: Ultrafast electron diffraction

- Structural dynamics
- Resolve atomic length and time scales: ~1 Å, ~100 fs

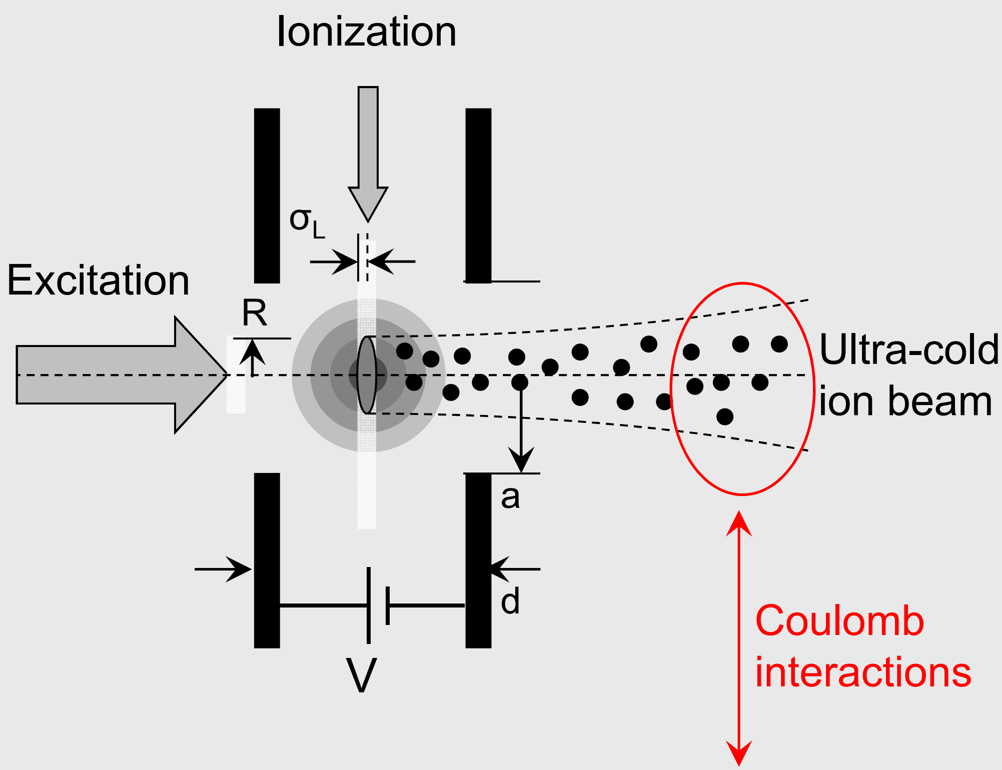


Application: Focused ion beams (FIB)



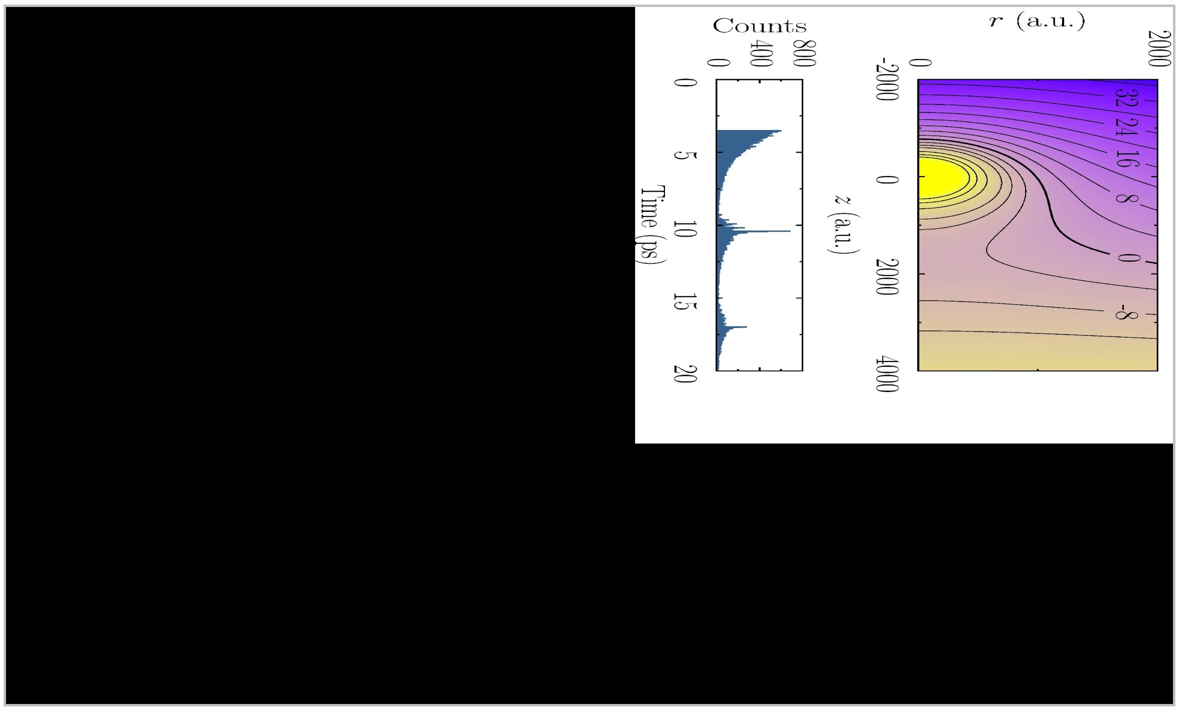
http://www.s3.infm.it/fib.html

Laser-cooled ion source



MOT parameters	
Temperature:	200 μK
v_{th}	0.22 m/s
n	10^{18} m^{-3}
Typical current:	10 pA
R	13 μm
σ_L	1.4 μm
Geometry	
V	2 kV
d	20 mm
a	1 mm

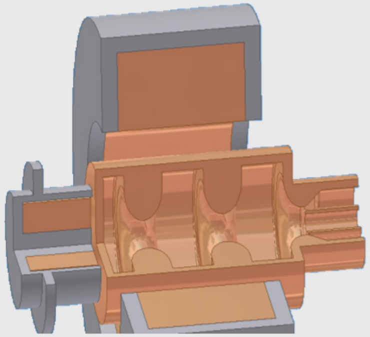
Simple theory predicts total collapse of brightness
But that is without acceleration…



Click into window and wait for movie to start

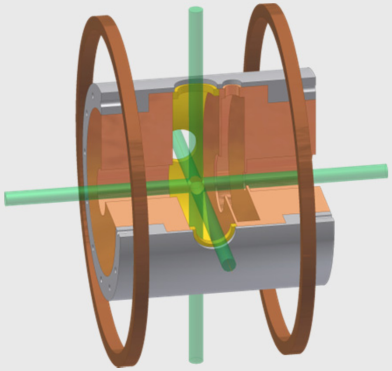
Movie: Wouter Engelen

Brighter sources, better simulations



Photogun: for example DESY / LCLS:

- Initial emittance ~ 1 µm (eV energy spread)
- Emittance ~ preserved in entire device
- Required simulation accuracy: <1 µm



Laser-cooled sources:

- Initial emittance: < 1 nm (meV energy spread)
- Emittance?
- Desired simulation accuracy: <1 nm

Quantum degenerate sources

- …

‘Typical’ simulation code: GPT

Tracks sample particles in time-domain

- Relativistic equations of motion
- Fully 3D, including all non-linear effects

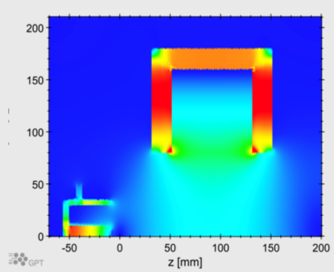
- GPT solves with 5th order embedded Runge Kutta, adaptive stepsize
- GPT can track ~10^6 particles on a PC with 1 GB memory
- Challenge: E(r,t), B(r,t), flexibility without compromising accuracy

External fields

- Analytical expressions

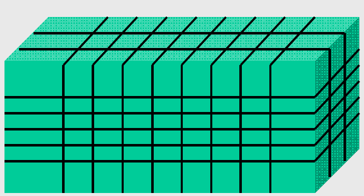
  {E,B}=f(x,y,z,t)

- Field-maps

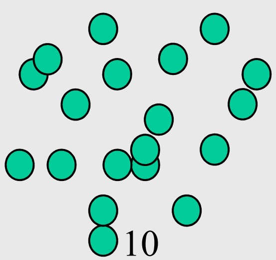


Coulomb interactions

- Particle in Cell



- All interactions



GPT Users Worldwide

www.pulsar.nl/gpt

48 Research institutes

Andrzej Soltan Institute for Nuclear Studies	Poland
Advanced Industrial Science and Technology (AIST)	Japan
Akita National College of Technology	Japan
Argonne National Laboratory (ANL)	USA
Bhabha Atomic Research Centre	India
Brookhaven National Laboratory	USA
Cells	Spain
Centre for Advanced Technology	India
Consorcio ESS BILBAO	Spain
Daresbury Laboratory	UK
Deutsches Electronen-Synchrotron (DESY)	Germany
European Synchrotron Radiation Facility (ESRF)	France
Fermi National Accelerator Laboratory (FN…	USA
FOM-Rijnhuizen	Netherlands
Forschungszentrum Jülich GmbH	Germany
Forschungszentrum Rossendorf (FZ…	German…
Helmholtz-Zentrum Berlin	Germa…
High Energy Accelerator Re…	Japan
Institute of Applied Electro…	Japa…
Institute of Modern Physic… -CAS)	Chin…
Interfacultair Reactor Instituut	Neth…
Japan Atomic Energy Agency (JAEA)	Japa…
Jefferson Laboratory	USA
Korea Atomic Energy Research Institute …)	Sou… a
Lawrence Berkeley National Laboratory	USA
Los Alamos National Laboratory (LANL)	USA
Marshall Space Flight Center (NASA)	USA
Max Born Institute	Ger…
Max-Planck-Institut für Quantenoptik (MP…	Germ…
Moscow Engineering Physics Institute (M…	Russi…
National Synchrotron Radiation Research … r	Taiwan
Naval Postgraduate School	USA
Netvision	Israel
Paul Scherrer Institute (PSI)	Switzerland
Pohang Accelerator Laboratory (POSTEC…)	South Korea
Rafael Laboratories	Israel
Rutherford Appleton Laboratory (RAL)	UK
Sincrotrone Trieste S.C.p.A.	Italy
Soltan Institute for Nuclear Studies	Poland
Stanford Linear Accelerator Center (SLAC)	USA
Sameer R&D of Govt. of India	India
Shanghai Institute of Applied Physics	China
Sincrotrone Trieste S.C.p.A.	Italy
Soreq Research Center	Israel
Stanford Linear Accelerator Center (SLAC)	USA
Tekniker	Spain
Tokyo Institute of Technology	Japan
TRIUMF	Canada

9 Commercial companies

Bharat Electronics Ltd.	India
Biosterile Technologies	Russia
FEI Company	Netherlands
Hitachi	Japan
Ishikawajima-Harima Heavy Industries	Japan
Kobe Steel, Ltd.	Japan
Océ Printing Systems	Germany
Positronics Research	USA
Sumitomo Heavy Industries	Japan

43 Universities

Abertay Dundee	UK
Ankara University	Turkey
Australian National University	Australia
Cornell University	USA
Delft University of Technology	Netherlands
Technische Universität Darmstadt	Germany
Eindhoven University of T… E)	Netherlands
Florida State Universit…	USA
Groningen Univers…	Netherlands
…roshima Univer…	Japan
…erial College	UK
…nnes Gute… Universität Mainz	Germany
… Universi…	Japan
…gpook Na… University	South Korea
…rsity of C… a at Los Angeles (UCLA	USA
…n Unive… llege	UK
…hester U… ty	UK
…urne U…	Australia
…l Univers…	Canada
…hen Univ…	Germany
…ya Univer…	Japan
…raska – Lin… iversity	USA
…egen Unive…	Netherlands
Osaka University	Japan
Oxford University	UK
Paris – sud University	France
Sichuan University	China
Stanford University	USA
Strathclyde	UK
Technische Universität Darmstadt	Germany
Tel Aviv University	Israel
Tohoku University	Japan
Tokyo University	Japan
Toronto University	Canada
Tsukuba University	Japan
Tsinghua University	China
Twente University	Netherlands
University of Abertay Dundee	UK
University of Strathclyde	UK

100

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Coulomb interactions

Macroscopic:

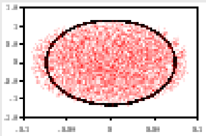
- Space-charge
- Average repulsion force
- Bunch expands
- Deformations in phase-space
- Governed by Poisson's equation

Microscopic:

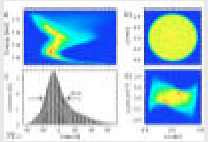
- Disorder induced heating
- Neighbouring particles 'see' each other
- Potential energy → momentum spread
- Stochastic effect
- Governed by point-to-point interactions

GPT simulations

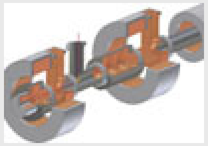
PRL 93, 094802
O.J. Luiten et. al.



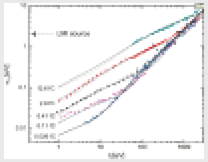
JAP 102, 093501
T. van Oudheusden et. al.



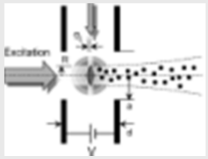
PRST-AB 9, 044203
S.B. van der Geer et. al.



PRL 102, 034802
M. P. Reijnders et. al.

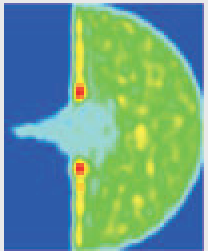


JAP 102, 094312
S.B. van der Geer et. al.



Nature Photonics
Vol 2, May 2008
M. Centurion et. al.

And many others…



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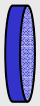
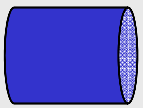
Particle-Mesh (in-Cell)



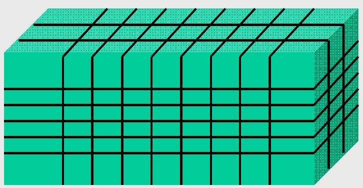
Bunch in laboratory frame

- <u>Mesh-based electrostatic solver in rest-frame</u>



Bunch in rest frame

- Bunch is tracked in laboratory frame
- Calculations in rest-frame $z' \approx \gamma\, z, \gamma = 1 \big/ \sqrt{1 - v^2/c^2}$



Meshlines

- Mesh
  – Density follows beam density
  – Trilinear interpolation to obtain charge density

ρ' Charge density

$-\nabla^2 V' = \rho'/\varepsilon_0$ Poisson equation

- Solve Poisson equation

$\mathbf{E}' = -\nabla V' \quad \mathbf{B}' = 0$ Interpolation

- 2nd order interpolation for the electrostatic field E'

$\{\mathbf{E},\mathbf{B}\} = \mathrm{L}(\mathbf{E}')$ Lorentz transformation to laboratory frame

- Transform E' to E and B in laboratory frame

Coulomb interactions

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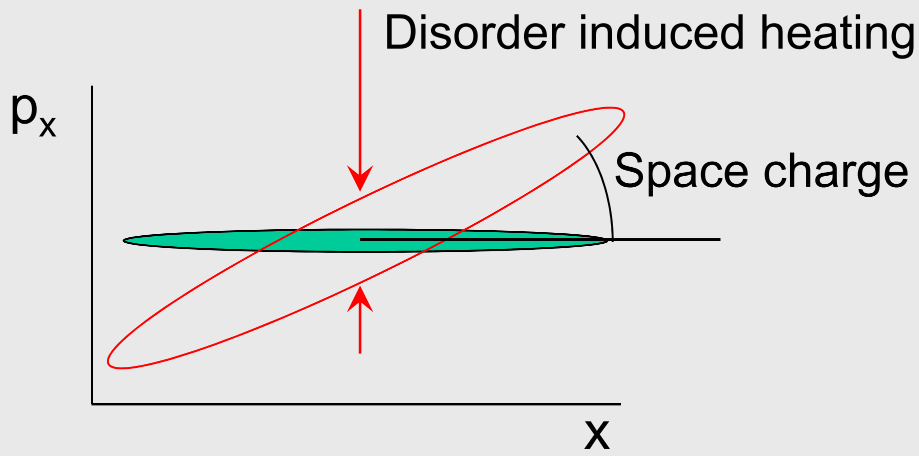

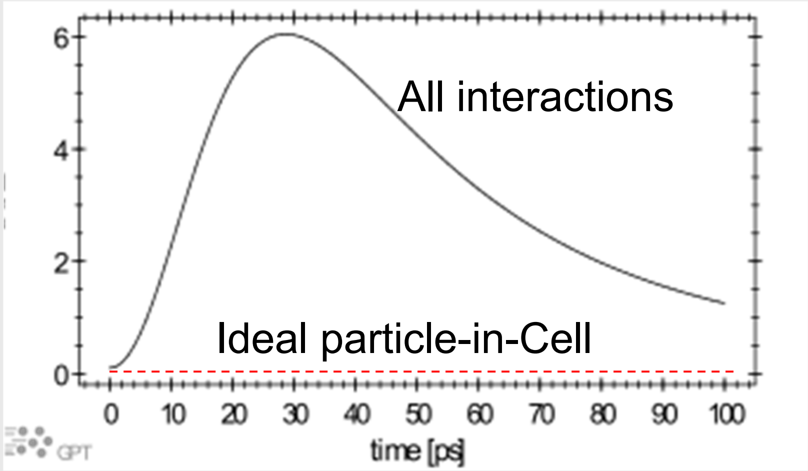

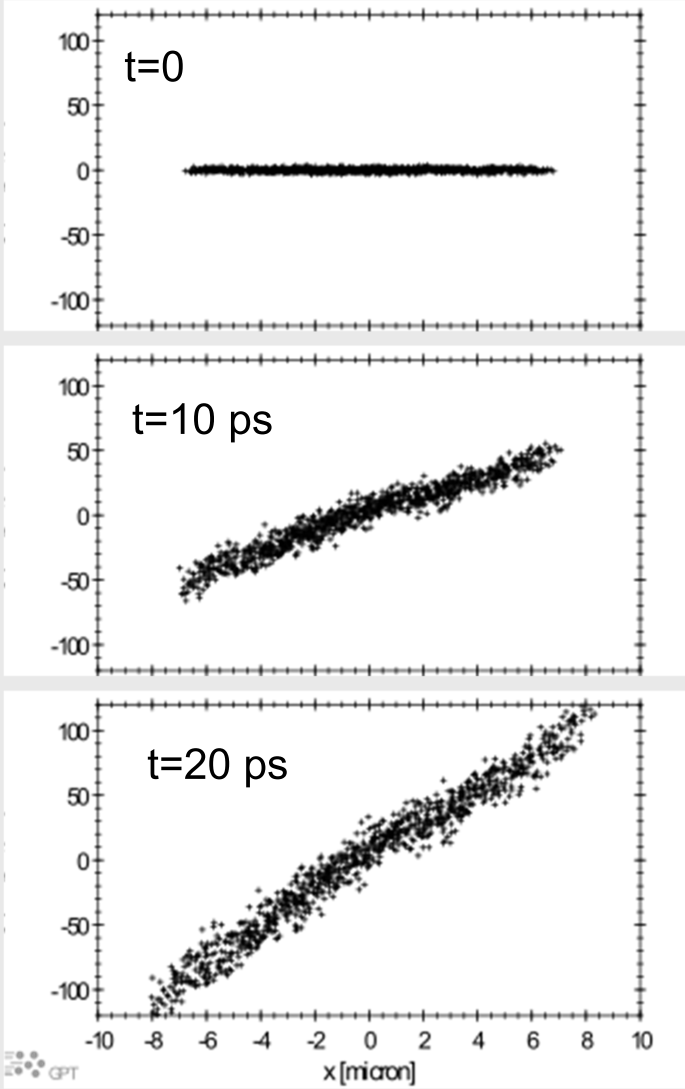

GPT simulations: $n=10^{18}$ m^{-3}

Analogy of a cold beam

Rhône Glacier 2012: Bas van der Geer

We need to go inside

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Disorder induced heating

Random processes

↓

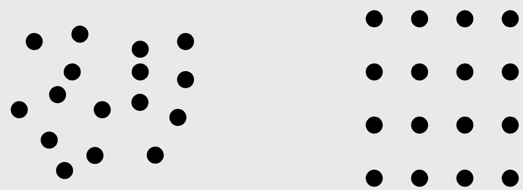
Excess potential energy U

↓ Coulomb interactions

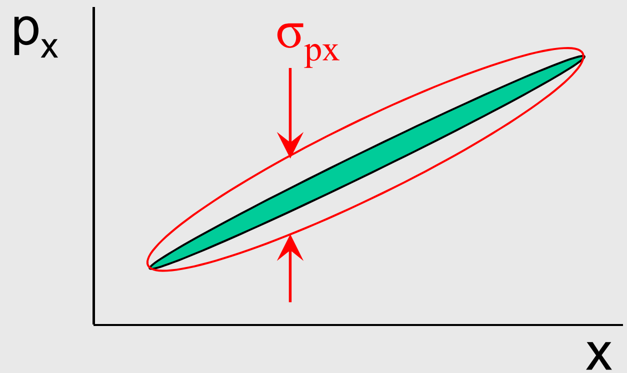
Momentum spread

↓

Temperature ↑
Brightness ↓



High U   Low U



$$\left.\begin{aligned}\sigma_{p_x} &= \sqrt{m\,k\,T_x}\\ &= mc\frac{\varepsilon_x}{\sigma_x}\end{aligned}\right\} \Rightarrow T_x = \frac{mc^2}{k}\frac{\varepsilon_x^2}{\sigma_x^2}$$

$$B_\perp = \frac{J}{\pi\,k\,T}$$

Paradigm shift

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Photo/thermionic emission

Space-charge

- ‘Shaping’ the beam
- Ellipsoidal bunches

Particle-in-Cell

- Macro-particles
- One species
- Fluid assumption
- Liouville holds
- Convergent rms values

Laser cooled sources

Disorder induced heating

- Fast acceleration
- Breaking randomness

Tree-codes (B&H, FMM, P^3M)

- Every particle matters
- Ions and electrons
- Ab initio
- No Liouville to the rescue
- Divergent rms values

$$k\,T_{\text{photogun}} \gg 0.02\, n^{1/3}\, q^2 / \varepsilon_0 \gg k\,T_{\text{laser-cooled}}$$

Algorithms…

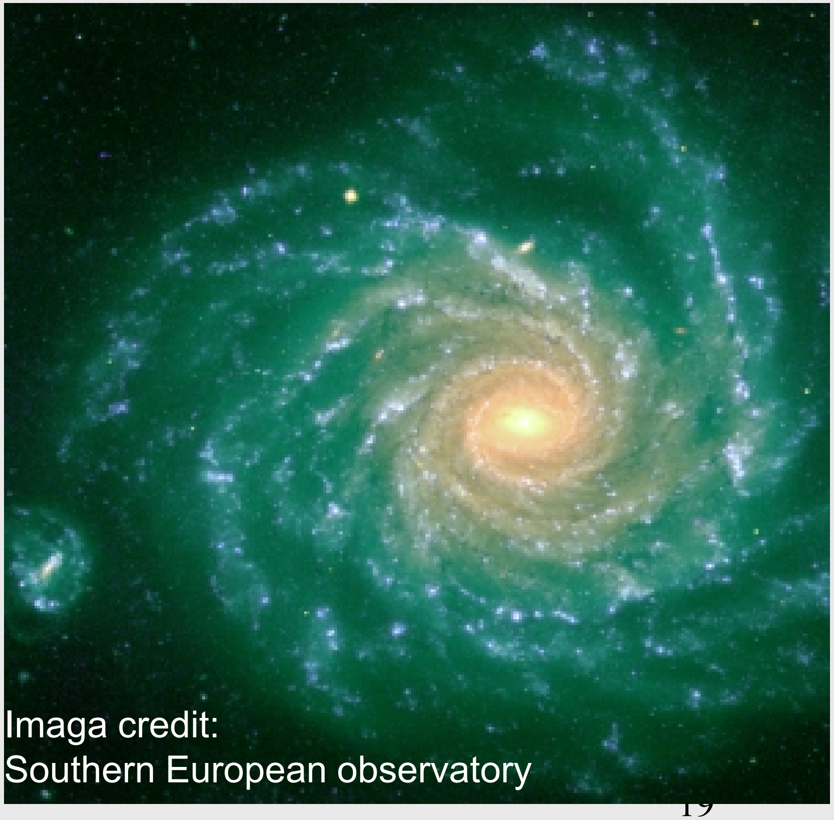
All interactions $O(N^2)$:

- PP Particle-Particle → slow
- P^3M Particle-Particle Particle-Mesh

Accuracy traded for speed:

- B&H Barnes&hut tree: O(N log N)
- FMM Fast-Multipole-Method: O(N)

- …



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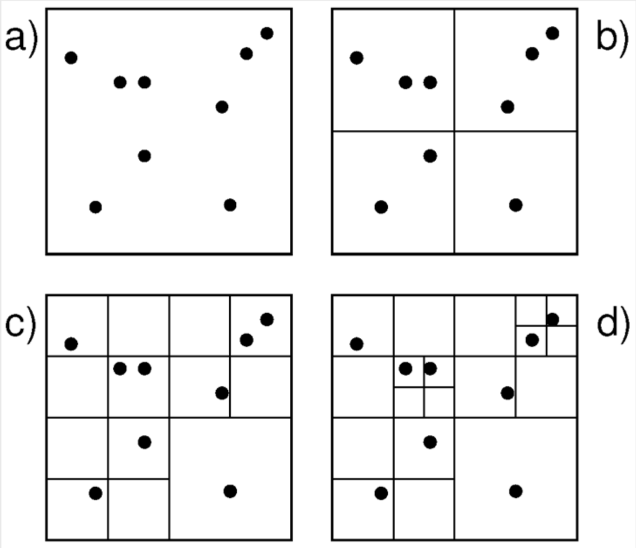
Barnes-Hut

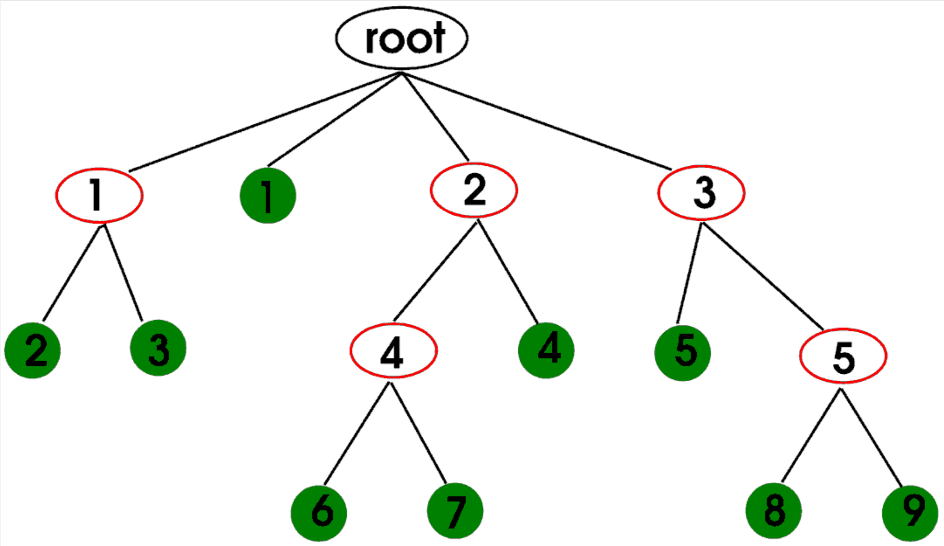
Hierarchical tree algorithm:

- Includes all Coulomb interactions
- O(N log N) in CPU time
- User-selectable accuracy

Division of space



Tree data structure



J. Barnes and P. Hut, Nature 324, (1986) p. 446.

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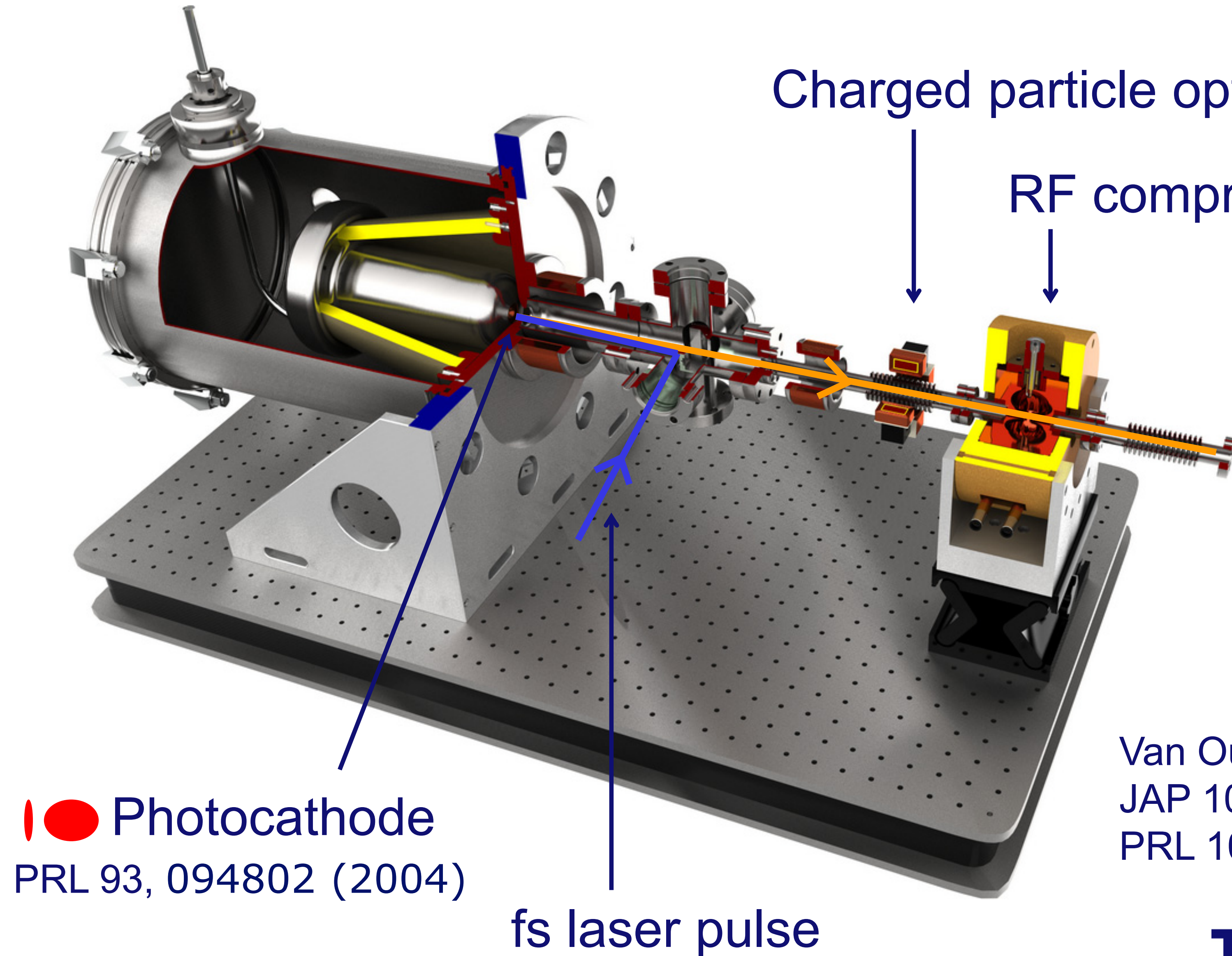
Barnes-Hut: GPT 3.1 implementation

- C++
- RAII (Resource Acquisition Is Initialization)
  - Entire tree is created in constructor
  - Exception handling to free resources in case of failure
- Constructor can create different classes for subnodes
  - For different hardware (GPU, different processor, ...)
  - For different distributions (one outlier, single species, ...)
  - Factory design pattern
- Single-thread construction, parallel traversal
- TODO: Minimize memory management overhead
  - Boost pool allocators

Single-shot Electron Diffraction

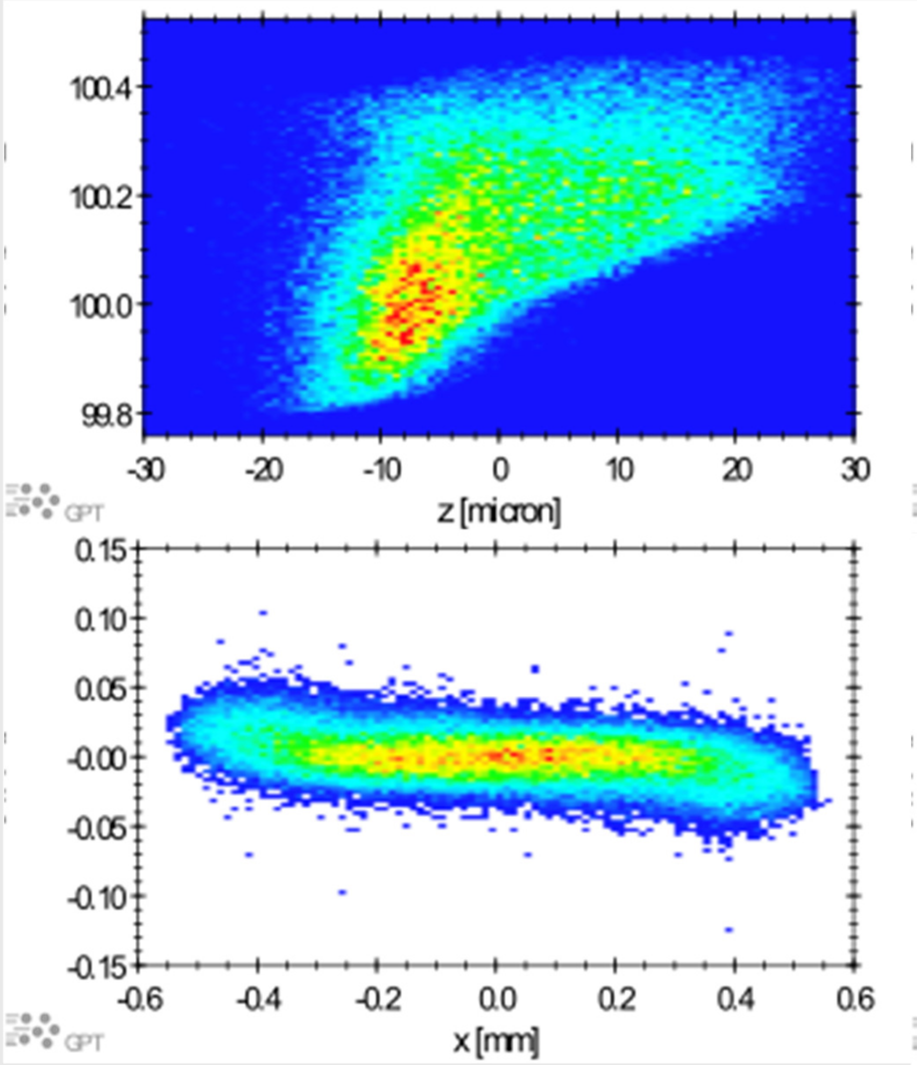


Van Oudheusden et al.,
JAP 102, 093501 (2007)
PRL 105, 264801 (2010)

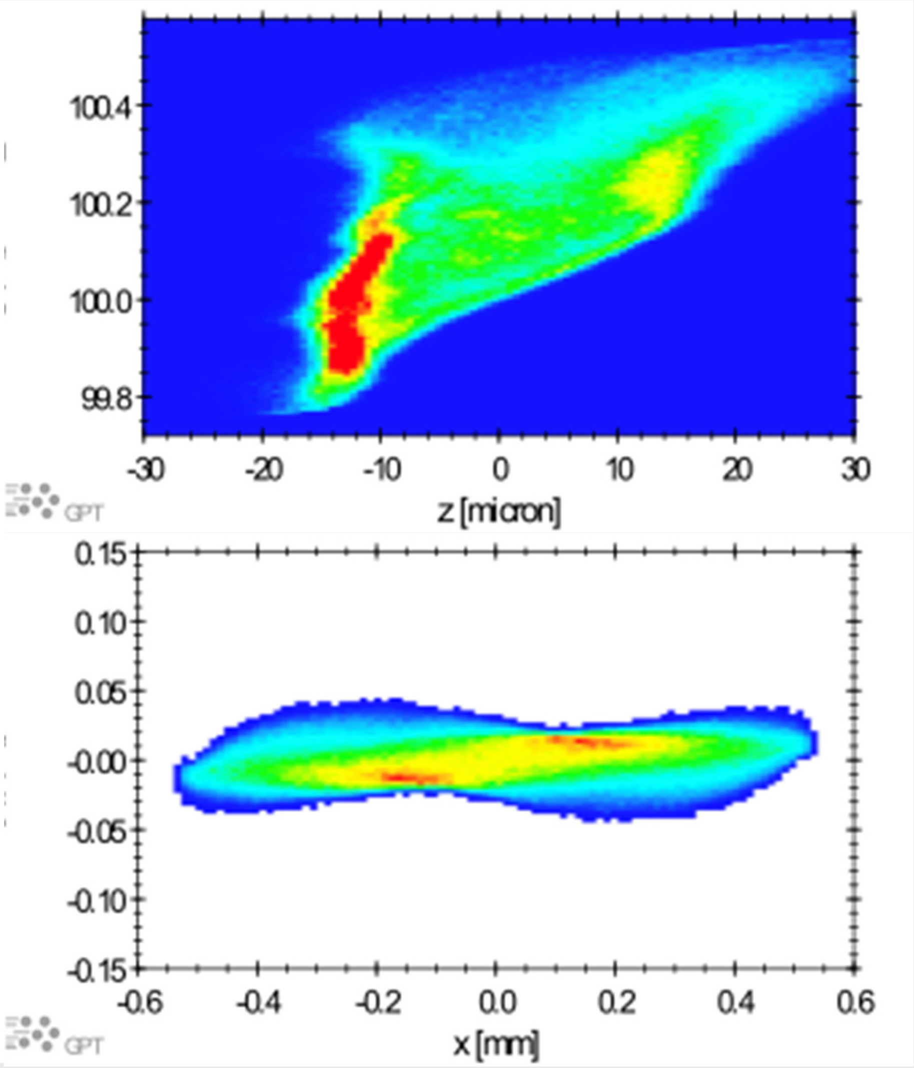
TU/e Technische Universiteit Eindhoven University of Technology

UED: Tree versus PIC model in GPT

Tree (all interactions)



PIC (Poisson solver)



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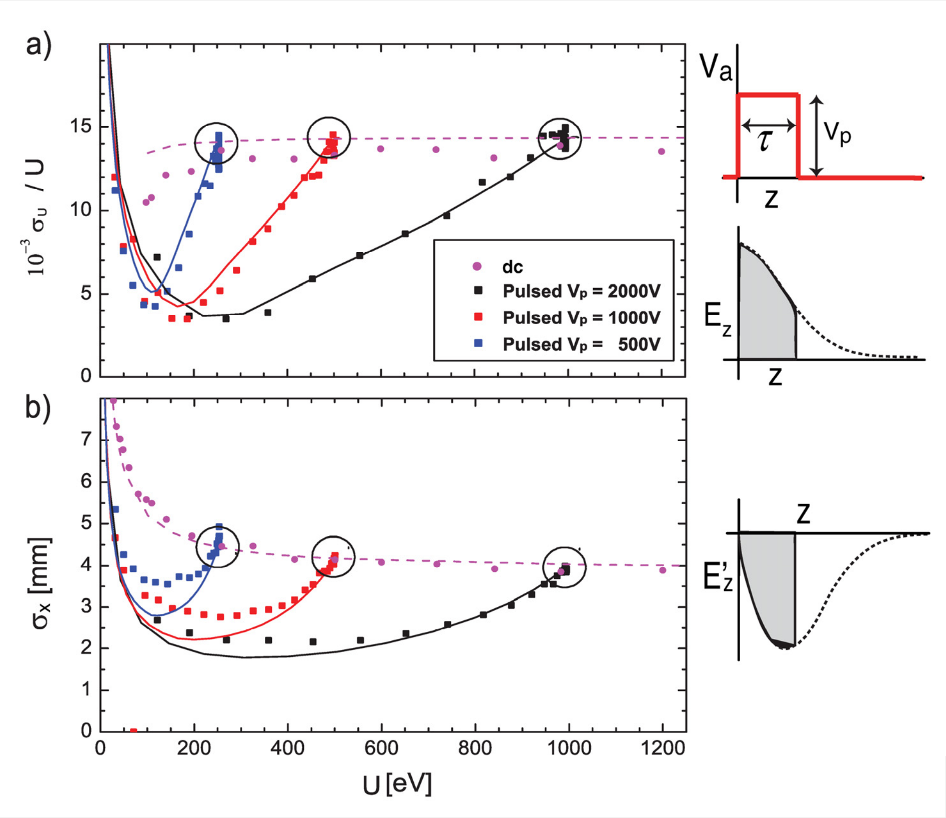
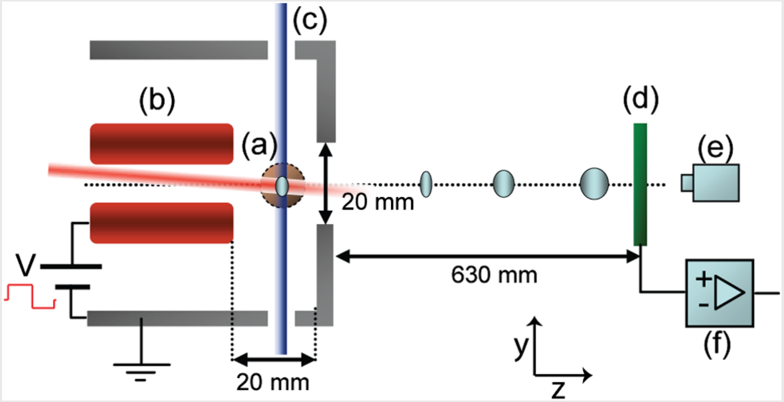
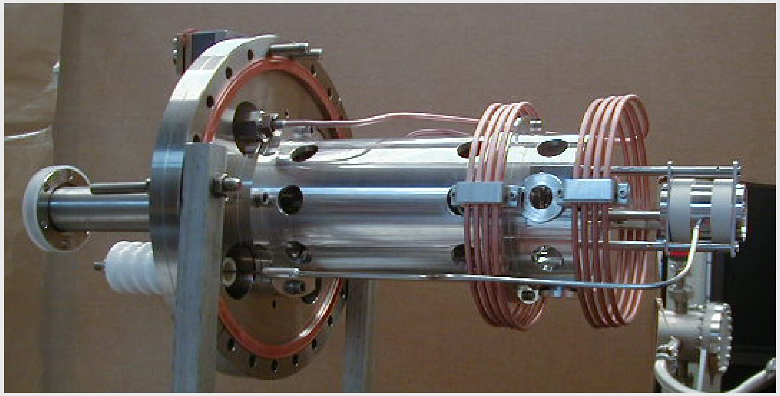
Comparison with experiments







M. P. Reijnders, N. Debernardi, S. B. van der Geer, P.H.A. Mutsaers, E. J. D. Vredenbregt, and O. J. Luiten,
Phase-Space Manipulation of Ultracold Ion Bunches with Time-Dependent Fields
PRL 105, 034802 (2010).

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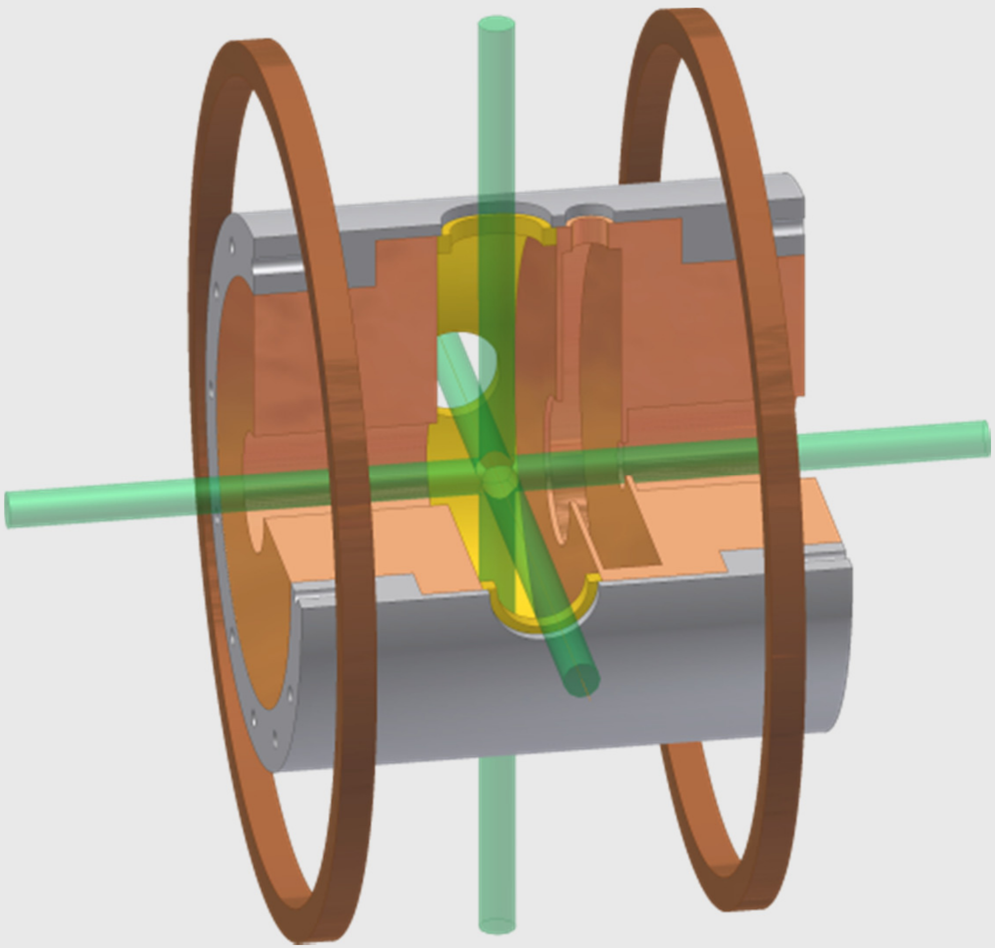
Laser-cooled e^- source



Fields:

Cavity field	20 MV/m rf-cavity
DC offset	3 MV/m

Particles:

Charge	0.1 pC (625k e^-)
Initial density	10^{18} / m^3
Ionization time	10 ps
Initial Temp	1 K

GPT tracking:

- All particles
- Realistic fields
- All interactions

Longitudinal emission dynamics

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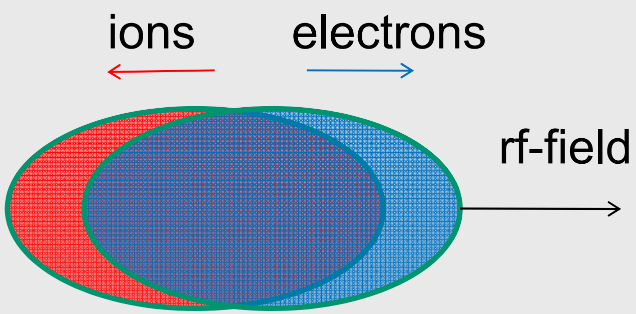
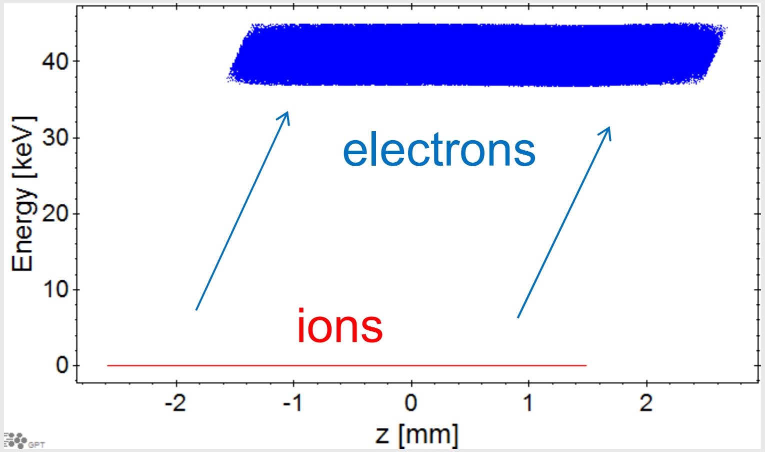
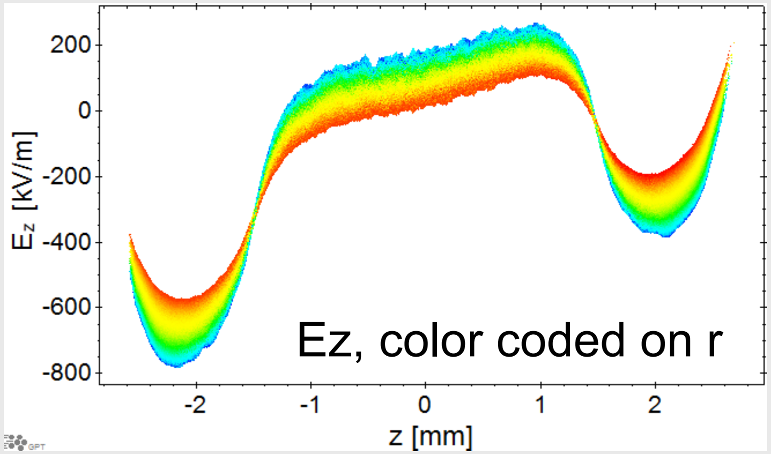
Longitudinal acceleration

- rf field
- Combined spacecharge



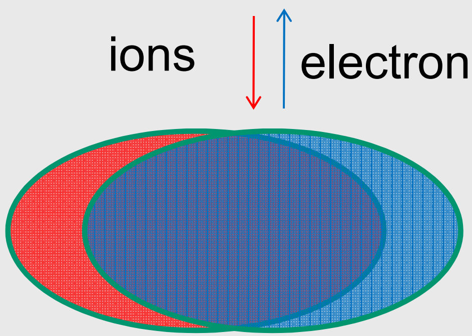


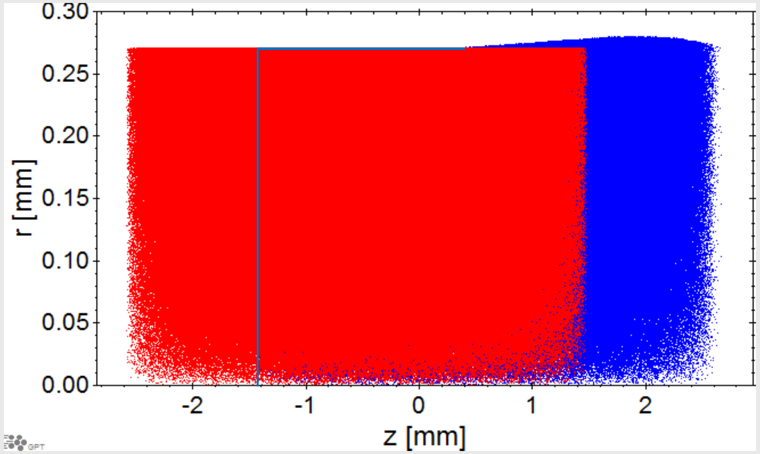


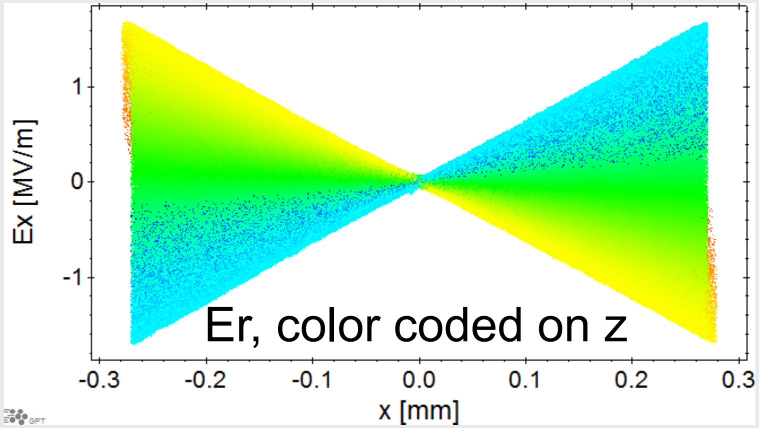
Transverse emission dynamics

Transverse acceleration

- While new ones are still being ionized
- While ions keep them together







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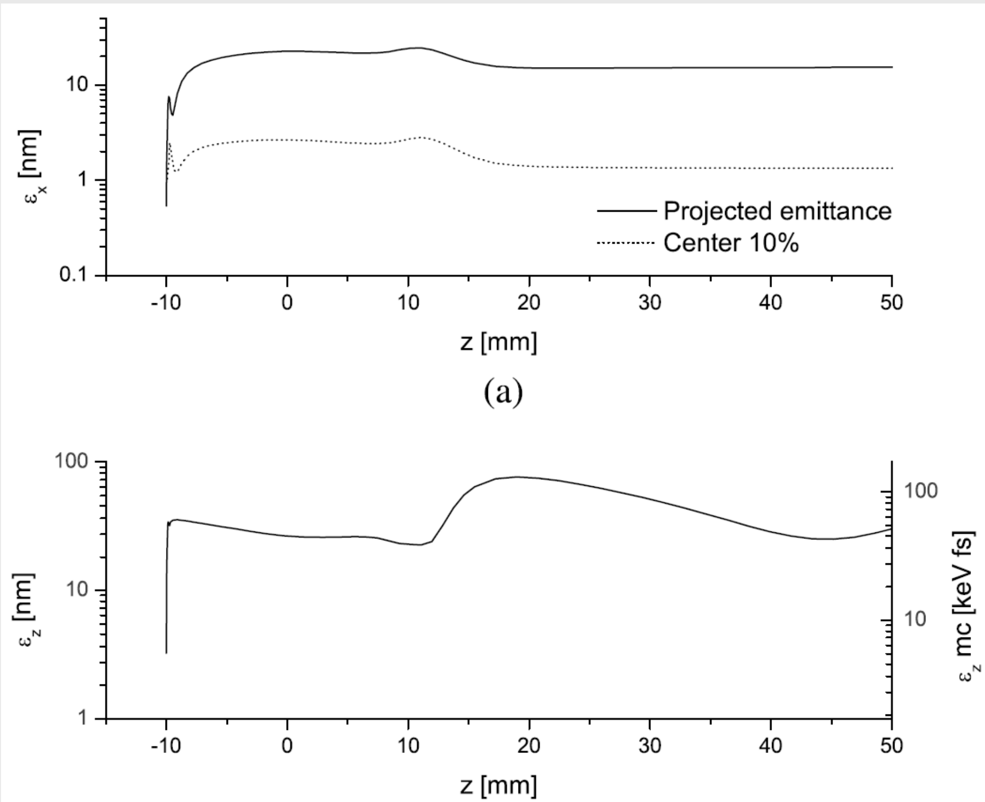
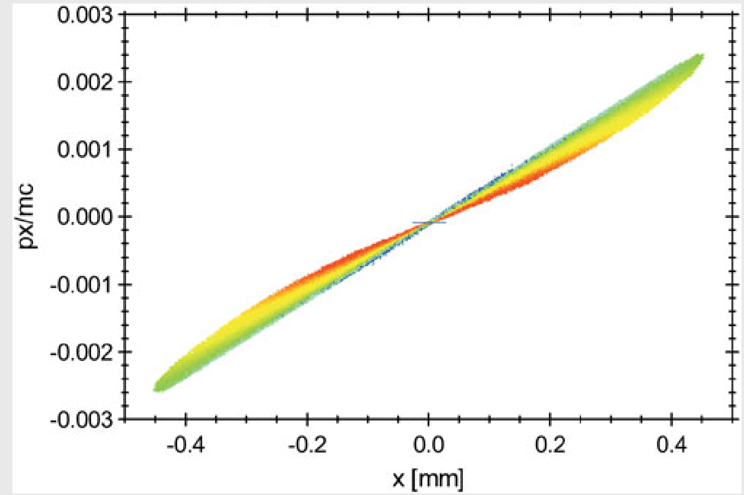
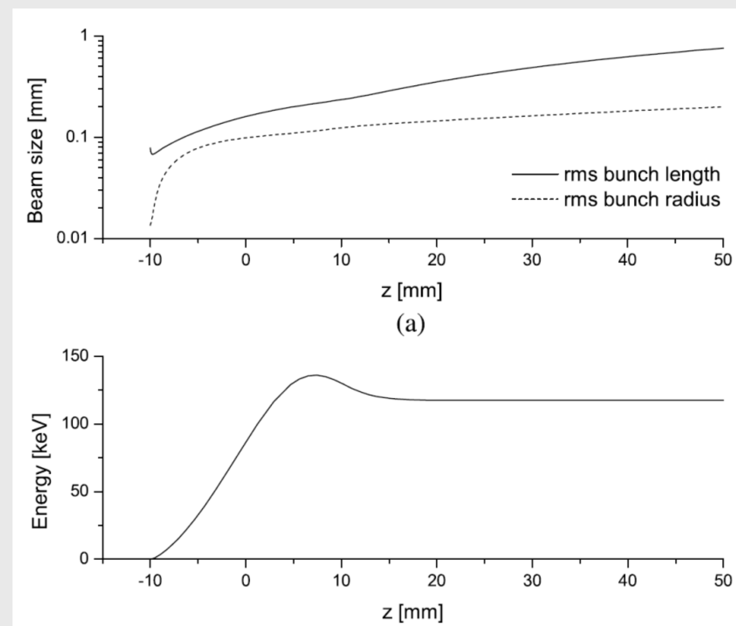
Laser cooled e⁻ diffraction



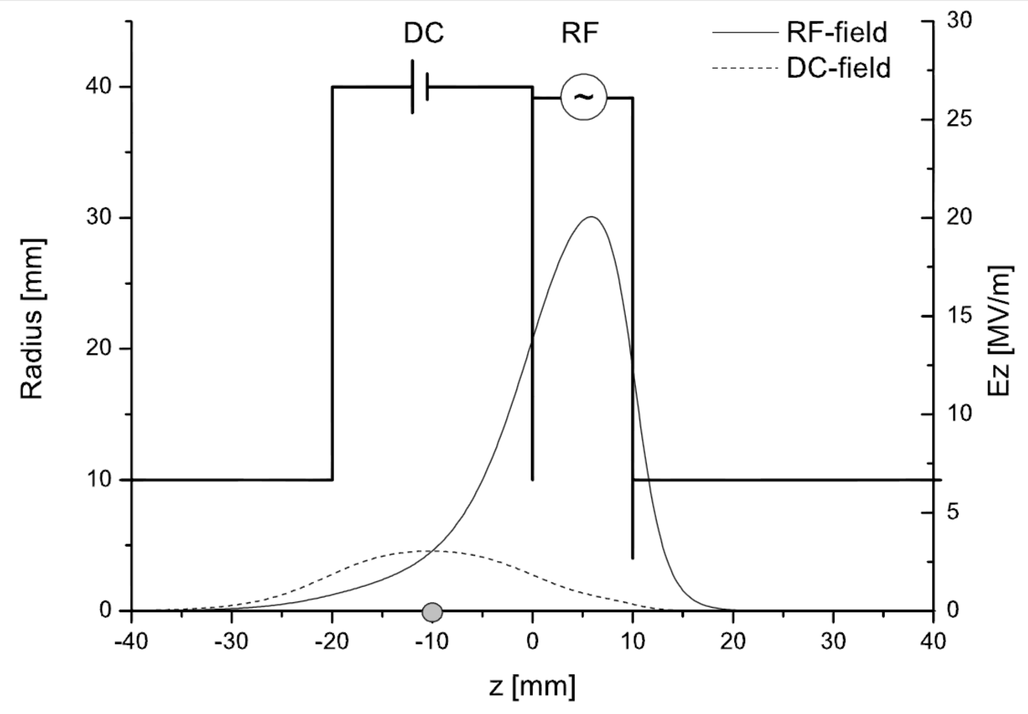




GPT Simulations include:

- Realistic external fields
- Start as function of time and position
- Relativistic equations of motion
- All pair-wise interactions included

Laser cooled e⁻ diffraction



GPT results:

ε_x	20 nm (rms)
10% slice	~1 nm
Energy	120 keV
Spread	1%
ε_z	60 keV fs
Charge	0.1 pC
	(625,000 e^-)

Ultracold Electron Source for Single-Shot, Ultrafast Electron Diffraction
Microscopy and Microanalysis 15, p. 282-289 (2009).
S.B. van der Geer, M.J. de Loos, E.J.D. Vredenbregt, and O.J. Luiten

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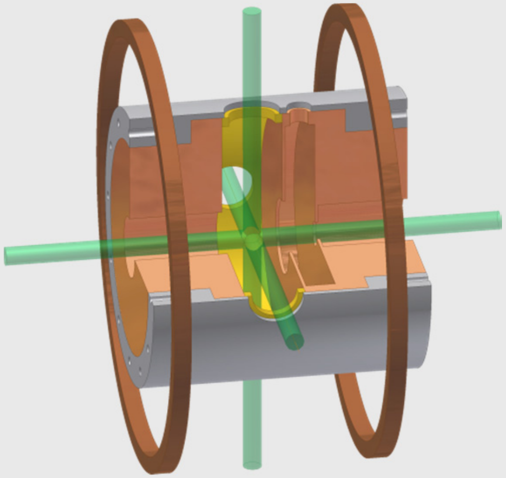
Conclusion



Laser-cooled sources:

- Very promising new development
- Experimental results match (GPT) predictions
- Bright future

Higher brightness:

- Requires new simulation techniques
  for the calculation of all pair-wise Coulomb interactions
- Such as implemented in GPT where we can now track >1M particles including all pair-wise interactions
- Produces phase-space distributions with divergent rms values

Globular cluster Messier 2 by Hubble Space Telescope. Located in the constellation of Aquarius, also known as NGC 7089.
M2 contains about a million stars and is located in the halo of our Milky Way galaxy.

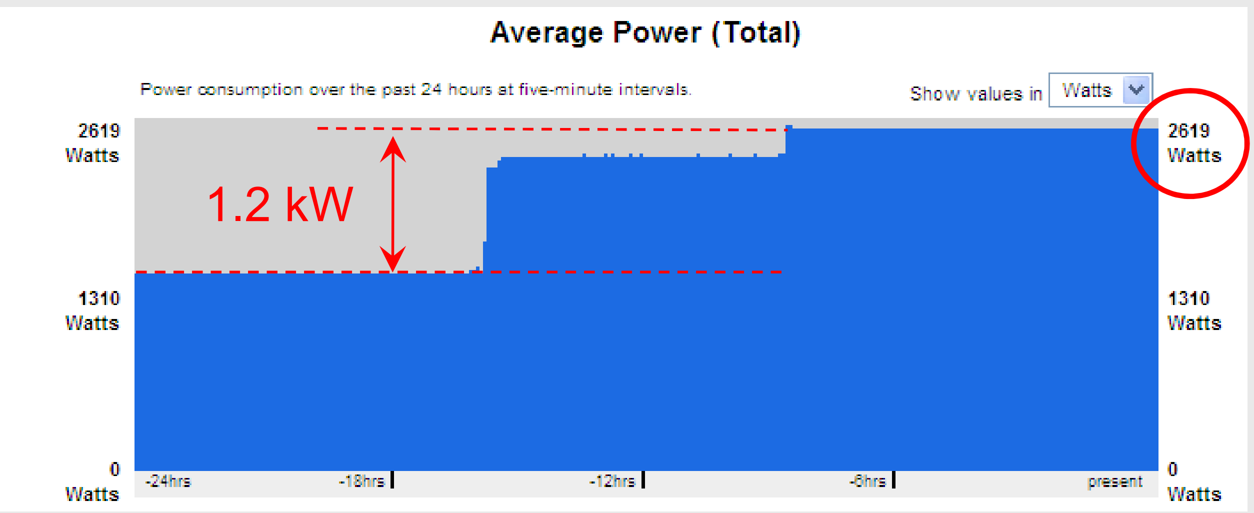
GPT hardware requirements

GPT kernel:

- Programming language: C and C++
- Multi-core functionality: openMP
- Distributed scans: MPI

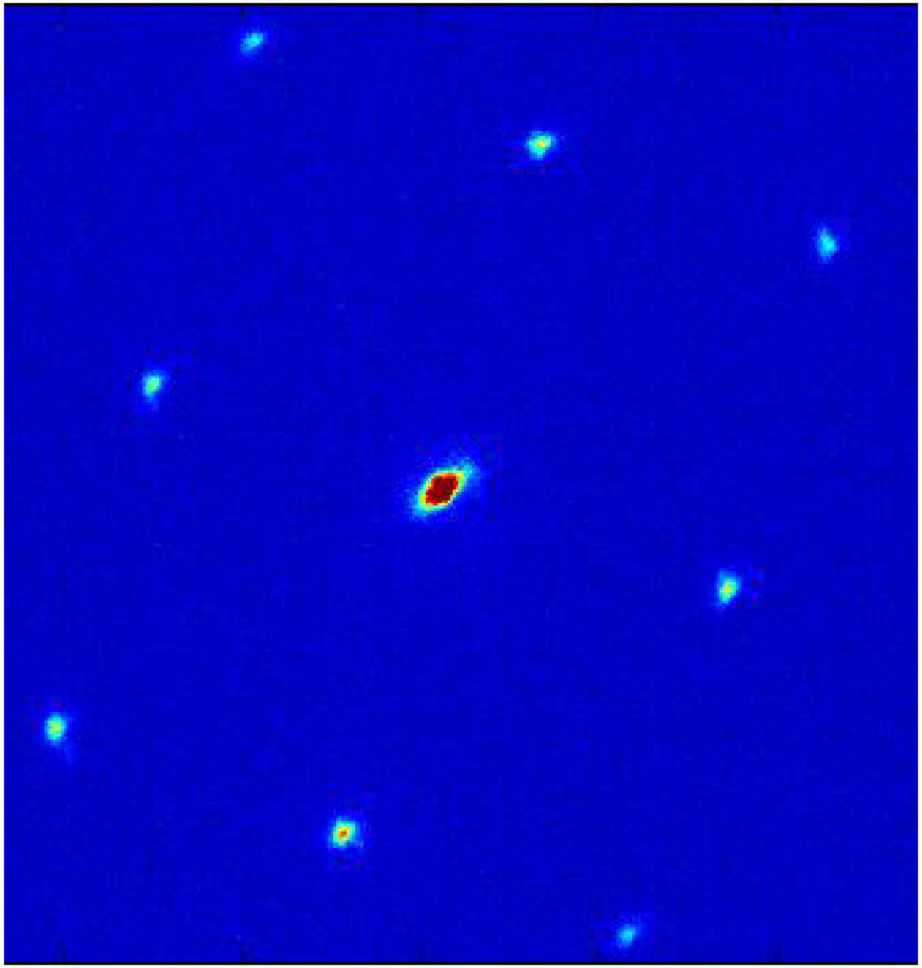
Mac mini

If you can run Microsoft Office, you can track ~1M particles



HP blade server: 16 servers, 128 cores, 1.2 kW of GPT power!

Single-shot Diffraction Pattern



Monocrystalline Au
U = 100 keV
Q = 400 fC
σ_{spot} = 200 μm

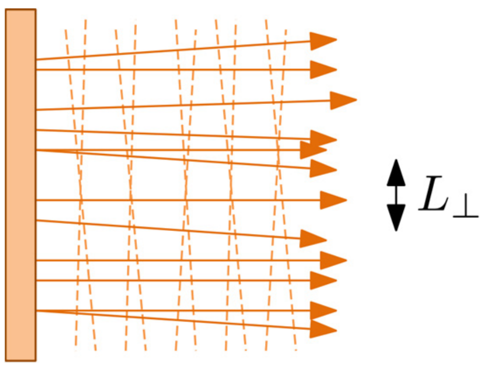
Spot analysis:
$L_{\perp} \approx 3$ nm

Study macromolecules:
mm sized crystals!?
… or a better source

Technische Universiteit Eindhoven University of Technology

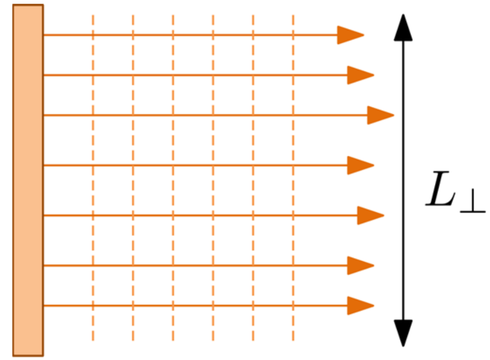
New Concept Electron Source

Photoemission source

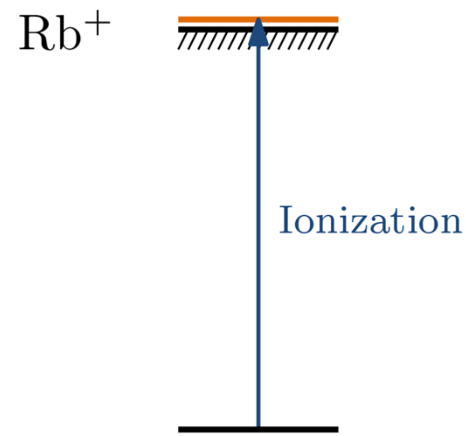


σ_E = 0.5 eV
T = 5000 K

Ultracold source



T = 10 K!



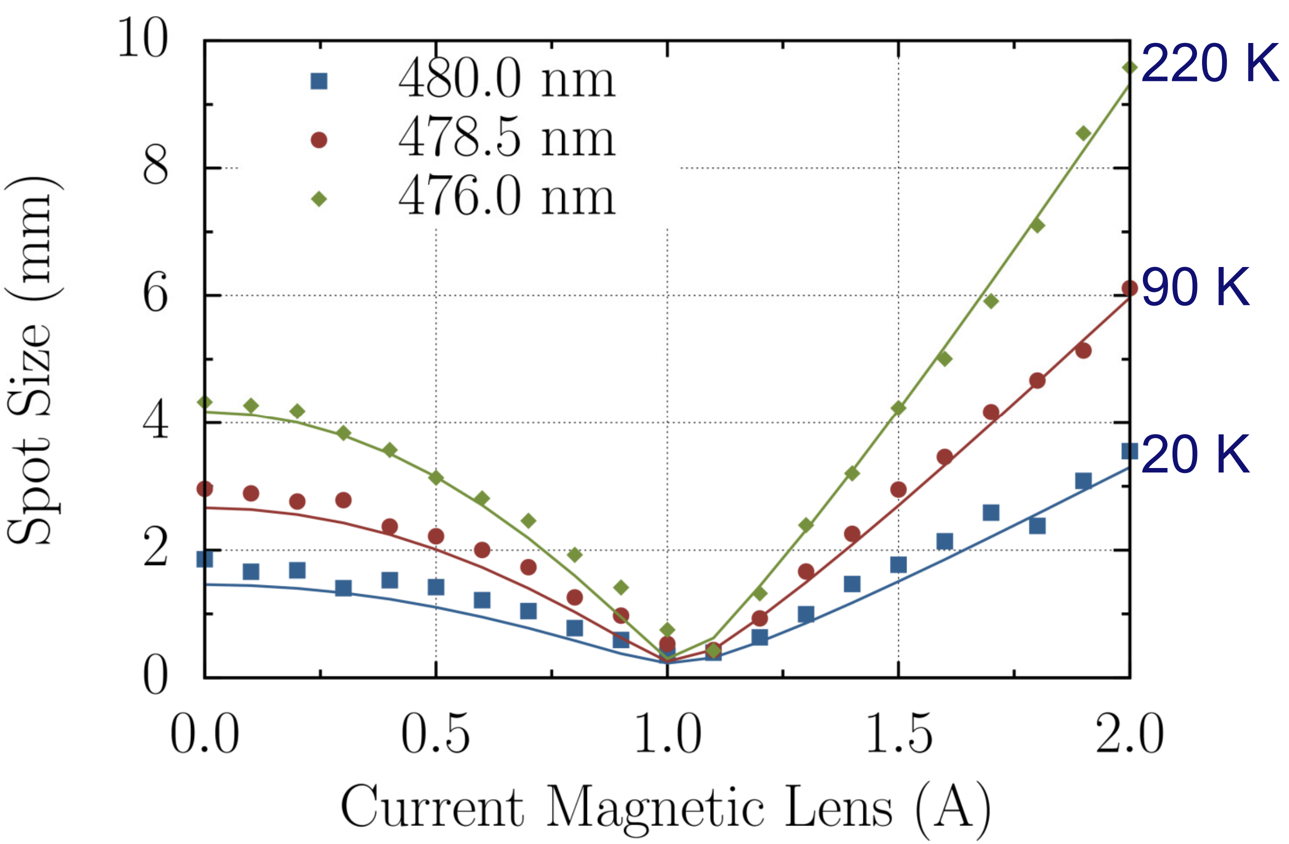
Near-threshold photoionization

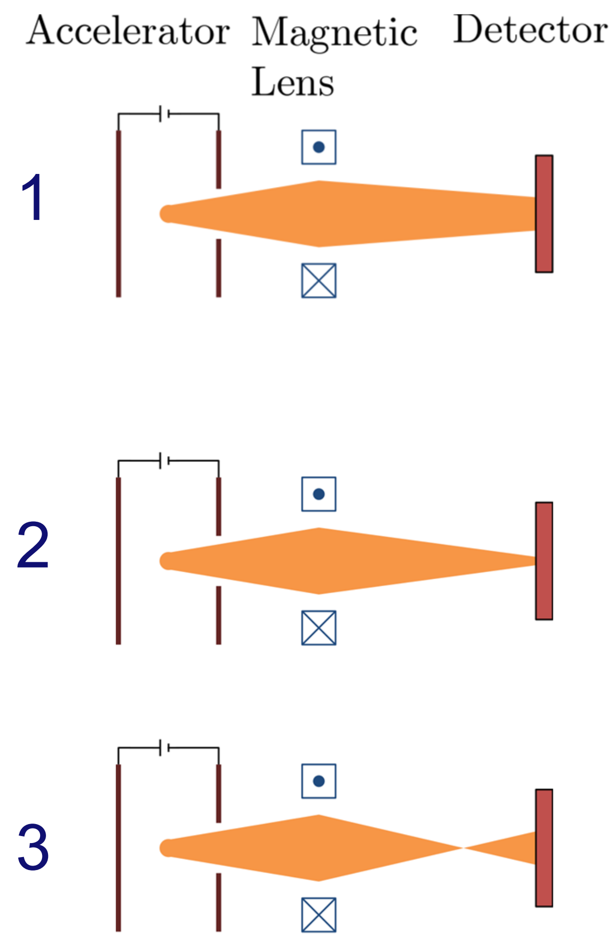
Angular spread $\sigma_\theta = \sqrt{\frac{kT}{2U}}$

Coherence length $L_\perp = \frac{\lambda}{2\pi\sigma_\theta}$

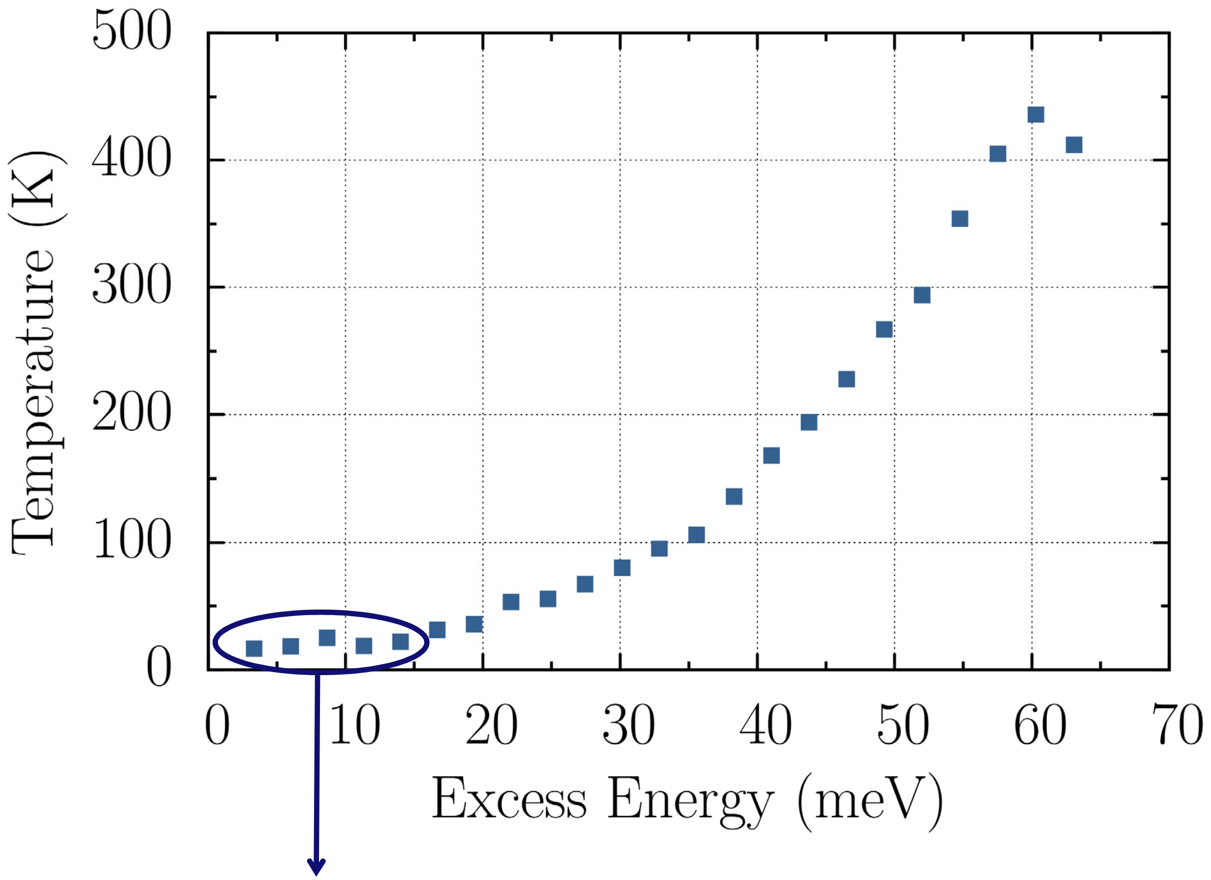
Taban et al.,
EPL 91, 46004 (2010)

Measure T with Waist Scan





Temperature vs. Excess Energy

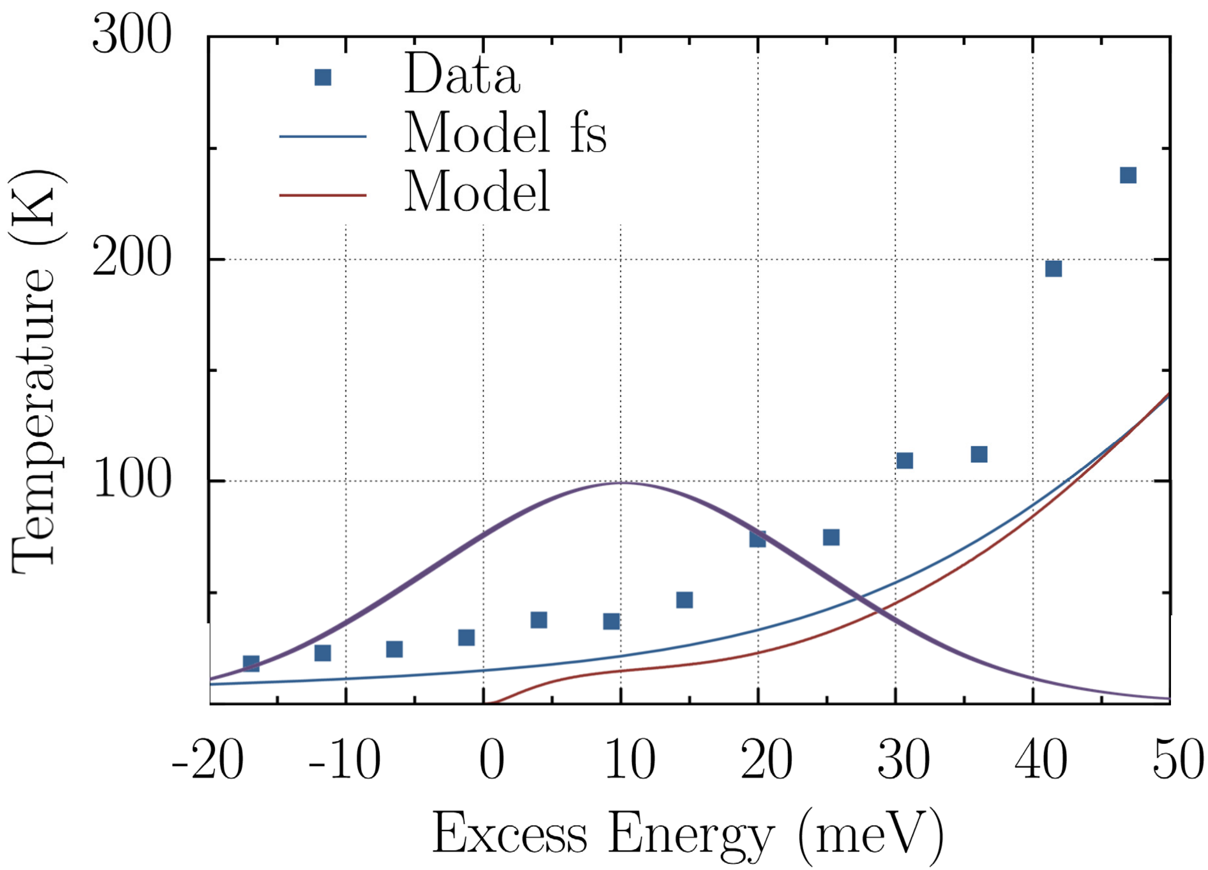


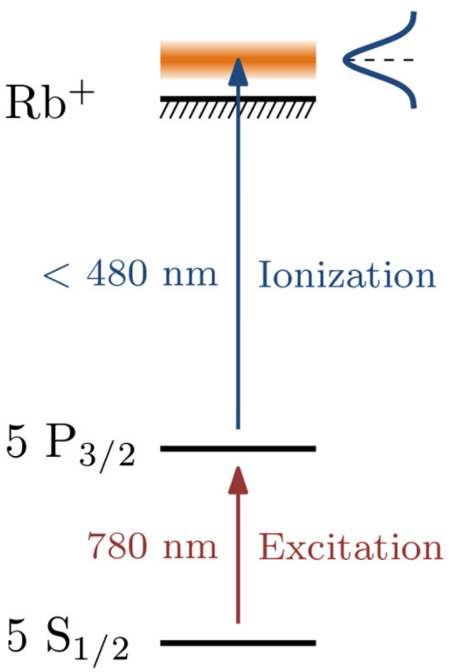
T = 20 K!

$L_\perp$ = 40 nm @ 200 µm spot

Technische Universiteit Eindhoven University of Technology

Comparison Measurement with Model

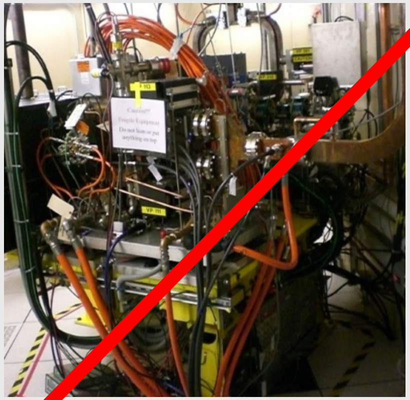




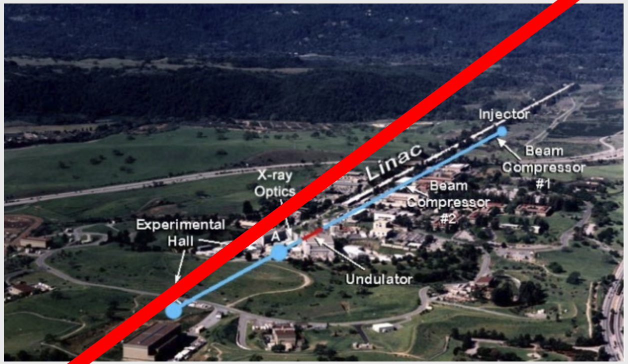
Ultracold ✓

Ultrafast (?)

Miniaturized DESY/LCLS ??



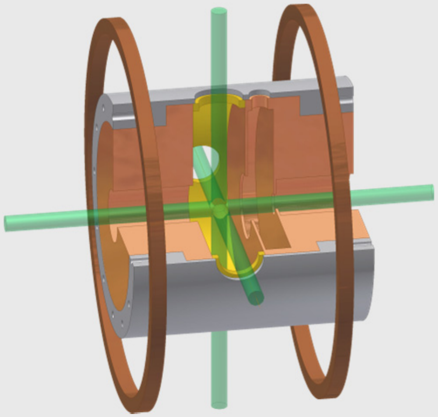
RF-photogun



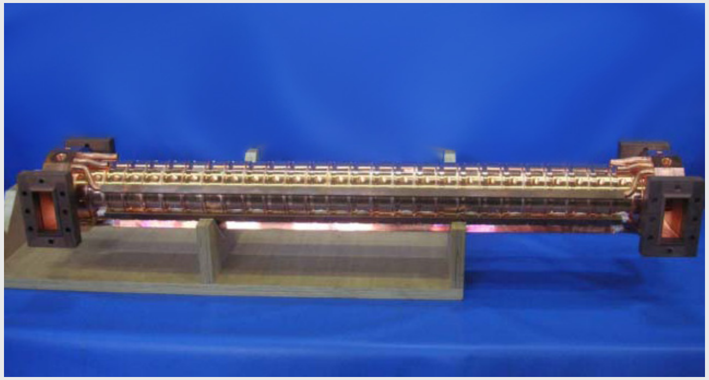
GeV Accelerator

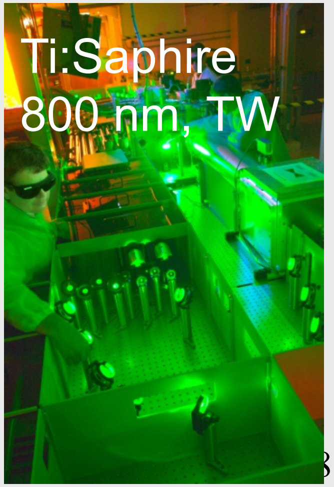
Undulator

laser-cooled source



MeV accelerator





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FEL equations

$$\frac{\varepsilon_n}{\gamma} = \frac{\lambda_{rad}}{4\pi} \qquad \lambda_{rad} = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right) \qquad \bar{\rho} = \rho\,\frac{mc\gamma}{\hbar k} = \frac{\sigma(p_z)}{\hbar k}$$

$$L_g = \frac{1}{\sqrt{3}}\sqrt[3]{\frac{2mc\gamma^3\sigma^2\lambda_u}{\mu e K^2 I}} = \frac{4\pi\sigma^2}{\lambda_{rad}}$$

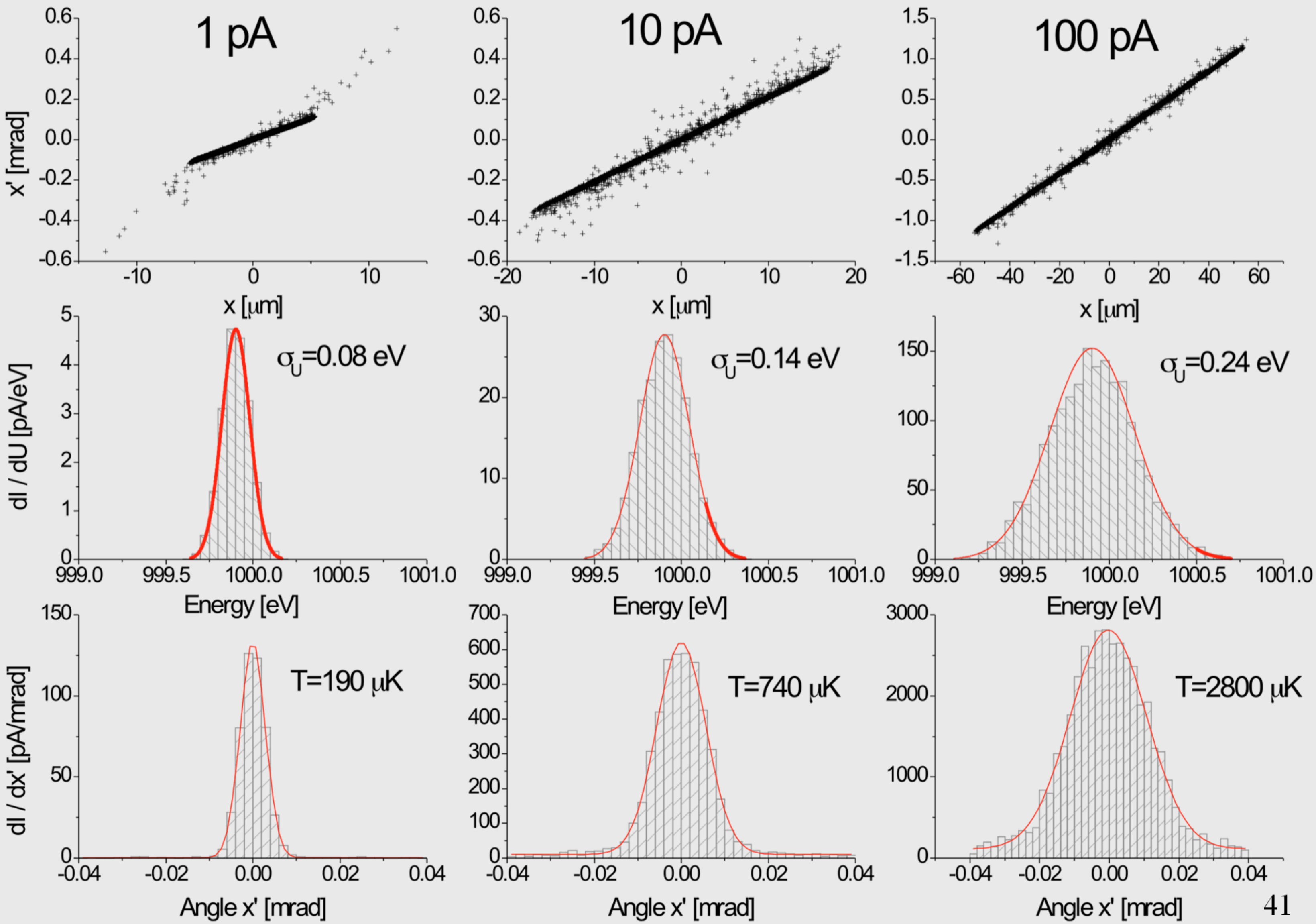
$$\rho_{FEL} = \frac{1}{4\pi\sqrt{3}}\frac{\lambda_u}{L_g} \qquad P = \gamma\,\frac{mc^2}{e} I\,\rho_{FEL}$$

$$\sigma_W = \frac{\rho_{FEL}}{2}\gamma\,\frac{mc^2}{e} \qquad I_{\max} = \frac{Q}{\varepsilon_z / \sigma_W}$$

FEL driven by laser-cooled source

Charge	1 pC	0.1 pC
Slice emittance	13 nm	1 nm
Longitudinal emittance	1 keV ps	0.1 keV ps
Peak current	100 A	1 mA
Energy	1.3 GeV	15 MeV
Undulator strength	0.1	0.5
λ_U	1.3 mm	800 nm
ρ_{FEL}	0.0002	0.00002
$\rho_{QUANTUM}$		0.1
Gain Length	0.28 m	2 mm
Wavelength	0.1 nm	0.4 nm
Power (1D)	25 MW	50 W, 60k photons

Direct GPT output

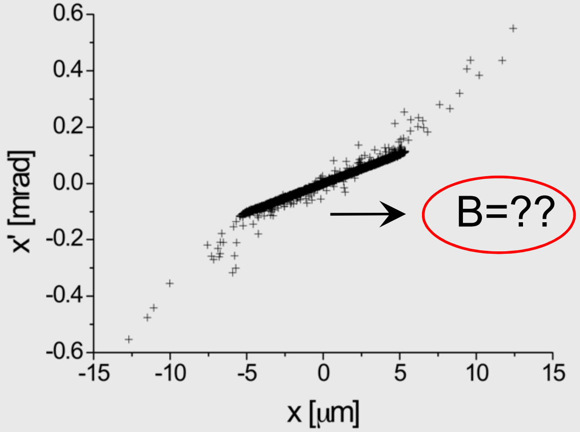


G. B. van der Geer, M. P. Reijnders, M. J. de Loos, E. J. D. Vredenbregt, P. H. A. Mutsaers, O. J. Luiten
Simulated performance of an ultracold ion source, JAP 102, 094312 2007

Phase-space density estimation

Problem:

- How to estimate (peak) brightness from a (4D) discrete distribution:



$$B_{reduced} = \frac{1}{V}\frac{d^2 I}{dA\, d\Omega}$$

$$= \frac{1}{\text{Volt}} \times \left(\frac{\text{Current [A]}}{\text{Phase space volume [m}^2\text{ rad}^2\text{]}} \right)$$

Volt → Normalization

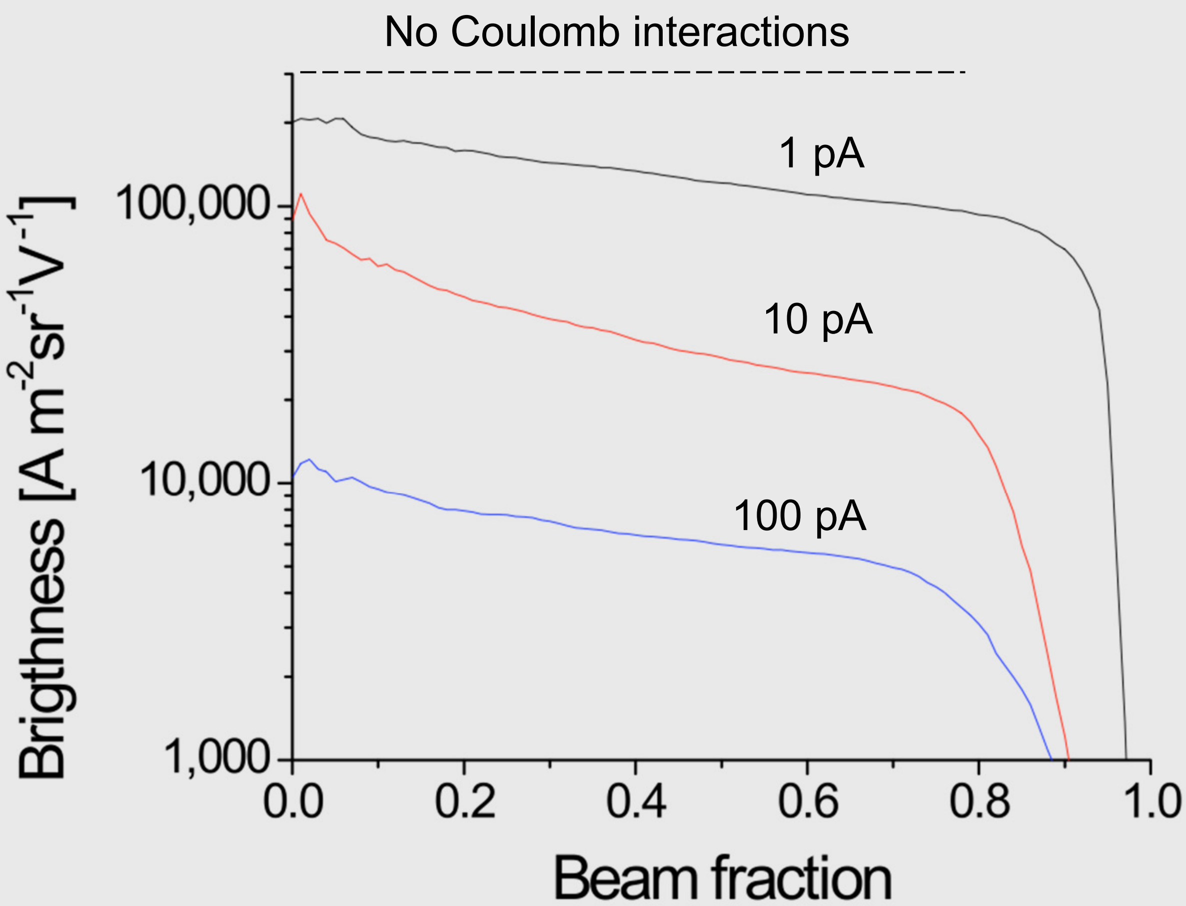
Phase space volume → ????

Proposed solution[1]:

- Count particles in (4D) hyper ellipsoid with orientation and aspect ratio given by beam sigma matrix

1 Inspired by: Eva Barbera Holzer, Figure of merit for muon cooling - an algorithm for counting particles in coupled phase-planes, NIM-A 532 (2004) 270-274.

Brightness as function of beam fraction



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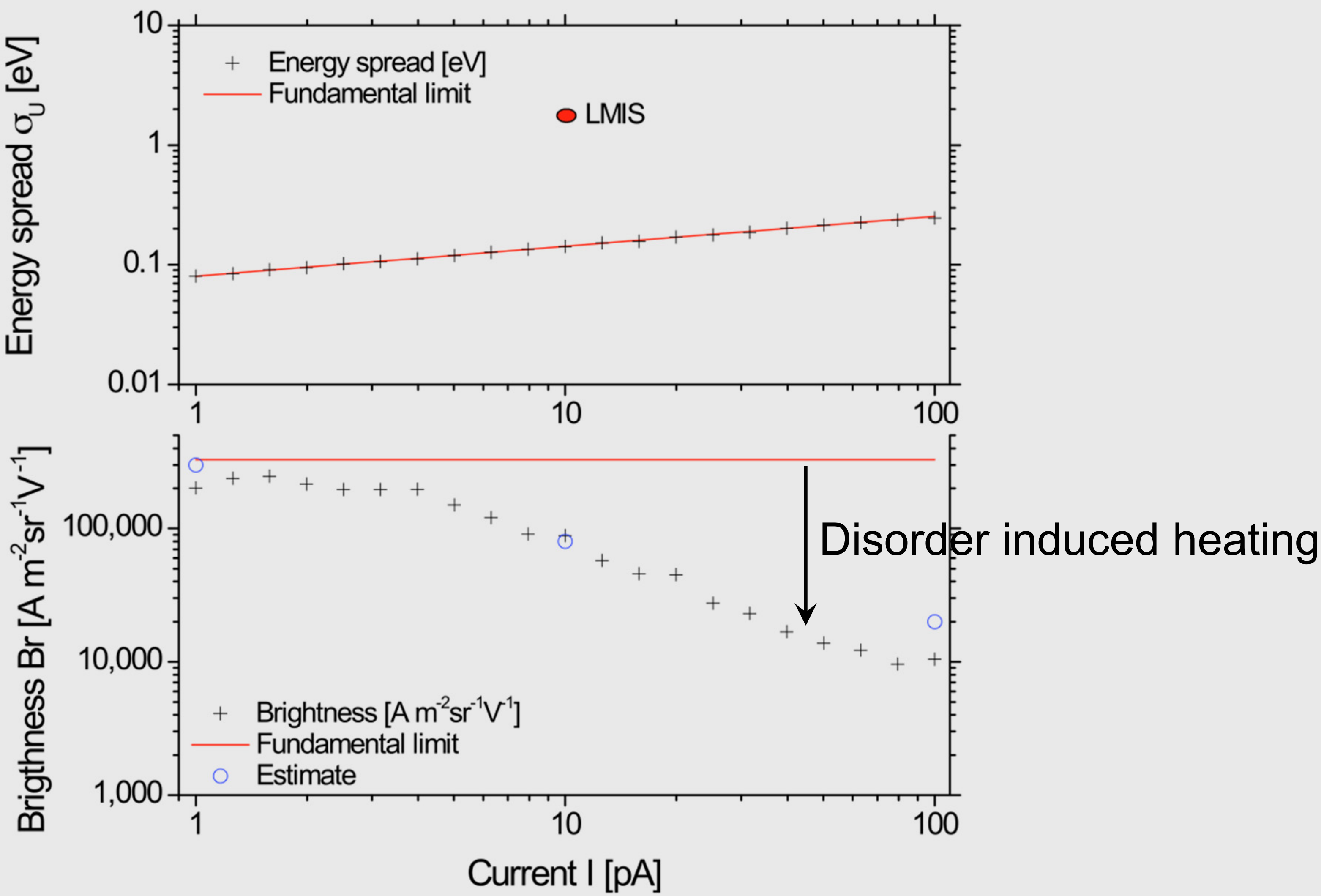
Simulated performance of an ultracold ion source, JAP 102, 094312 2007

Energy spread and brightness



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